

***pVT*-Second Virial Coefficients $B(T)$, Viscosity $\eta(T)$, and Self-Diffusion $\rho D(T)$ of the Gases: BF_3 , CF_4 , SiF_4 , CCl_4 , SiCl_4 , SF_6 , MoF_6 , WF_6 , UF_6 , $\text{C}(\text{CH}_3)_4$, and $\text{Si}(\text{CH}_3)_4$ Determined by Means of an Isotropic Temperature-Dependent Potential**

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We present results on self-consistent calculations of second pVT -virial coefficients $B(T)$, viscosity data $\eta(T)$, and diffusion coefficients $\rho D(T)$ for eleven heavy globular gases: boron trifluoride (BF_3), carbon tetrafluoride (CF_4), silicon tetrafluoride (SiF_4), carbon tetrachloride (CCl_4), silicon tetrachloride (SiCl_4), sulfur hexafluoride (SF_6), molybdenum hexafluoride (MoF_6), tungsten hexafluoride (WF_6), uranium hexafluoride (UF_6), tetramethyl methane ($\text{C}(\text{CH}_3)_4$, TMM), and tetramethyl silane ($\text{Si}(\text{CH}_3)_4$, TMS). The calculations are performed mainly in the temperature range between 200 and 900 K by means of isotropic $n-6$ potentials with temperature-dependent separation $r_m(T)$ and potential well depth $\varepsilon(T)$. The potential parameters at $T=0$ K (ε , r_m , n) and the enlargement of the first level radii δ are obtained solving an ill-posed problem of minimizing the squared deviations between experimental and calculated values normalized to their relative experimental error. The temperature dependence of the potential is obtained as a result of the influence of vibrational excitation on binary interactions. This concept of the isotropic temperature-dependent potential (ITDP) is presented in detail where gaseous SF_6 will serve as an example. The ITDP is subsequently applied to all other gases. This approach and the main part of the results presented here have already been published during 1996–2000. However, in some cases the data are upgraded due to the recently improved software (CF_4 , SF_6) and newly found experimental data (CF_4 , SiF_4 , CCl_4 , SF_6). © 2002 American Institute of Physics.

Key words: boron trifluoride; carbon tetrachloride; carbon tetrafluoride; molybdenum hexafluoride; silicon tetrachloride; silicon tetrafluoride; sulfur hexafluoride; tetramethyl methane; tetramethyl silane; transport and equilibrium properties of gases; tungsten hexafluoride; uranium hexafluoride.

Contents

List of Symbols.....	185	3.3.1. Sulfur hexafluoride, SF_6	189
1. Introduction.....	185	3.3.2. Molybdenum hexafluoride, MoF_6	190
2. Isotropic Temperature-Dependent Potential (ITDP).....	187	3.3.3. Tungsten hexafluoride, WF_6	190
3. Experimental Data.....	187	3.3.4. Uranium hexafluoride, UF_6	190
3.1. Planar Heavy Globular Molecules (BF_3)....	188	3.4. Tetramethyl Compounds $\text{C}(\text{CH}_3)_4$,	
3.2. Tetrahedral Heavy Globular Molecules (CF_4 , SiF_4 , CCl_4 , SiCl_4).....	188	$\text{Si}(\text{CH}_3)_4$	190
3.2.1. Carbon tetrafluoride, CF_4	188	3.4.1. Tetramethyl Methane, $\text{C}(\text{CH}_3)_4$	190
3.2.2. Silicon tetrafluoride, SiF_4	188	3.4.2. Tetramethyl Silane, $\text{Si}(\text{CH}_3)_4$	190
3.2.3. Carbon tetrachloride, CCl_4	188	4. Methodology.....	191
3.2.4. Silicon tetrachloride, SiCl_4	189	4.1. SF_6 as an Example.....	191
3.3. Octahedral Heavy Globular Molecules (SF_6 , MoF_6 , WF_6 , UF_6).....	189	4.1.1. Best Solution and Deviation Plots.....	191
		4.1.2. Comparison with Available B and η Calculations.....	192
		4.1.3. Comparison with the MMSV potential.....	194
		4.1.4. Summary.....	194
		5. Deviation Plots.....	194
		6. Tabulations.....	194

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7. Conclusion	198	24. Fit parameters according to Eqs. (6) and (7) for SiF ₄	203
8. Acknowledgments	215	25. Potential parameters $r_m(T)$ and $\varepsilon(T)$ and recommended thermophysical properties of CCl ₄	203
9. References	215	26. Fit parameters according to Eqs. (6) and (7) for CCl ₄	204
List of Tables			
1. BF ₃ . Set of experimental data used for approximation	188	27. Potential parameters $r_m(T)$ and $\varepsilon(T)$ and recommended thermophysical properties of SiCl ₄	205
2. CF ₄ . Set of experimental data used for approximation	188	28. Fit parameters according to Eqs. (6) and (7) for SiCl ₄	206
3. SiF ₄ . Set of experimental data used for approximation	188	29. Potential parameters $r_m(T)$ and $\varepsilon(T)$ and recommended thermophysical properties of SF ₆	206
4. CCl ₄ . Set of experimental data used for approximation	189	30. Fit parameters according to Eqs. (6) and (7) for SF ₆	207
5. SiCl ₄ . Set of experimental data used for approximation	189	31. Potential parameters $r_m(T)$ and $\varepsilon(T)$ and recommended thermophysical properties of MoF ₆	208
6. SF ₆ . Set of experimental data used for approximation	189	32. Fit parameters according to Eqs. (6) and (7) for MoF ₆	209
7. MoF ₆ . Set of experimental data used for approximation	190	33. Potential parameters $r_m(T)$ and $\varepsilon(T)$ and recommended thermophysical properties of WF ₆	209
8. WF ₆ . Set of experimental data used for approximation	190	34. Fit parameters according to Eqs. (6) and (7) for WF ₆	210
9. UF ₆ . Set of experimental data used for approximation	190	35. Potential parameters $r_m(T)$ and $\varepsilon(T)$ and recommended thermophysical properties of UF ₆	211
10. C(CH ₃) ₄ . Set of experimental data used for approximation	190	36. Fit parameters according to Eqs. (6) and (7) for UF ₆	212
11. Si(CH ₃) ₄ . Set of experimental data used for approximation	190	37. Potential parameters $r_m(T)$ and $\varepsilon(T)$ and recommended thermophysical properties of C(CH ₃) ₄	212
12. Normal vibrational frequencies and degeneracies (in parentheses) used in calculations: planar, tetrahedral, and octahedral molecules	191	38. Fit parameters according to Eqs. (6) and (7) for C(CH ₃) ₄	213
13. Normal vibrational frequencies and degeneracies (in parentheses) used in calculations: tetramethyl compounds	191	39. Potential parameters $r_m(T)$ and $\varepsilon(T)$ and recommended thermophysical properties of Si(CH ₃) ₄	214
14. The distribution of the RMS and $\langle R_i \rangle$ deviations of SF ₆ as a function of temperature	192	40. Fit parameters according to Eqs. (6) and (7) for Si(CH ₃) ₄	215
15. Influence of the change of the parameters PP on the RMS(PP) deviations normalized to the "best" solution deviation (RMS=0.657 a_{exp})	192		
16. The influence of the specific experimental data on our solution for SF ₆ ("jack-knife" check)	193		
17. Comparison between MMSV potential and ITDP	195		
18. ITDP parameters at T=0 K	198		
19. Potential parameters $r_m(T)$ and $\varepsilon(T)$ and recommended thermophysical properties of BF ₃	199	List of Figures	
20. Fit parameters according to Eqs. (6) and (7) for BF ₃	200	1. Weighted relative deviations of measured $B(T)$ and $\eta(T)$ of SF ₆ from the best solution obtained with the ITDP (zero line)	192
21. Potential parameters $r_m(T)$ and $\varepsilon(T)$ and recommended thermophysical properties of CF ₄	200	2. Relative deviations of the second pVT -virial coefficient for the individual experimental input data of SF ₆	193
22. Fit parameters according to Eqs. (6) and (7) for CF ₄	201	3. Relative deviations of the viscosity for the individual experimental input data of SF ₆	193
23. Potential parameters $r_m(T)$ and $\varepsilon(T)$ and recommended thermophysical properties of SiF ₄	202	4. Comparison of $\eta(T)$ calculated by means of ITDP (zero line) with the tabulated values of Boushehri <i>et al.</i> ²⁸ and Trengove and Wakeham. ²⁹ The deviations of the most accurate measurements used in the minimization	

are also plotted.....	194
5. Comparison of $B(T)$ calculated by means of ITDP (zero line) with the tabulated values of Boushehri <i>et al.</i> ²⁸	194
6. Comparison of the ITDP (at $T=300$ K and $T=600$ K) with the MMSV potential.....	194
7. Deviation plot for $B(T)$ of BF_3	195
8. Deviation plot for $B(T)$ of CF_4	195
9. Deviation plot for $B(T)$ of SiF_4	195
10. Deviation plot for $B(T)$ of CCl_4	195
11. Deviation plot for $B(T)$ of SiCl_4	196
12. Deviation plot for $B(T)$ of SF_6	196
13. Deviation plot for $B(T)$ of MoF_6	196
14. Deviation plot for $B(T)$ of WF_6	196
15. Deviation plot for $B(T)$ of UF_6	196
16. Deviation plot for $B(T)$ of $\text{C}(\text{CH}_3)_4$	196
17. Deviation plot for $B(T)$ of $\text{Si}(\text{CH}_3)_4$	196
18. Deviation plot for $\eta(T)$ of BF_3	196
19. Deviation plot for $\eta(T)$ of CF_4	197
20. Deviation plot for $\eta(T)$ of SiF_4	197
21. Deviation plot for $\eta(T)$ of CCl_4	197
22. Deviation plot for $\eta(T)$ of SiCl_4	197
23. Deviation plot for $\eta(T)$ of SF_6	197
24. Deviation plot for $\eta(T)$ of MoF_6	197
25. Deviation plot for $\eta(T)$ of WF_6	197
26. Deviation plot for $\eta(T)$ of UF_6	197
27. Deviation plot for $\eta(T)$ of $\text{C}(\text{CH}_3)_4$	198
28. Deviation plot for $\eta(T)$ of $\text{Si}(\text{CH}_3)_4$	198

List of Symbols

a_{exp}	relative experimental error
B	(pVT) second virial coefficient
β	acoustic second virial coefficient
C_k	enlargements of the highly excited states with respect to the enlargement of the first excited state
C_6	long-range dispersion constant
D	binary diffusion coefficient
F	sum of squared deviations between calculated and measured values
g_{vi}	degeneracy of vibrational state
h	Planck constant
k_B	Boltzmann constant
M	number of experimental input data
m	molecular weight
N	total number of normal vibrations
n	repulsive parameter
n_s	number of excited states
r	intermolecular distance
r_m	molecular separation in pair potential at $T=0$
$r_m^{(\text{eff})}$	molecular separation in pair potential at $T>0$
T	temperature
U	intermolecular interaction potential
x_k	relative population of the vibrational state
x_0	ground state relative population
δ	first vibrationally excited level enlargement
$\delta^{(\text{eff})}$	averaged enlargement of the molecular separation at $T>0$

ε	potential well depth at $T=0$
$\varepsilon^{(\text{eff})}$	potential well depth at $T>0$
η	viscosity
ρ	gas density
Z	vibrational partition function
ν	normal vibrational frequency
v_i	quantum number of the vibrationally excited level of i -th normal vibration
P	property ($B(T), \eta(T), \rho D(T)$)
PP	potential parameter ($r_m, \varepsilon, n, \delta$)

1. Introduction

Tables with reliable thermophysical data of heavy globular gases in a wide temperature range are requested in contemporary industry. For example, CF_4 , SiF_4 , CCl_4 , SiCl_4 , SF_6 , WF_6 , MoF_6 , $\text{C}(\text{CH}_3)_4$, and $\text{Si}(\text{CH}_3)_4$ are used in different microelectronic and chemical technologies (chemical vapor deposition, thin-film epitaxy, etc.). SF_6 and CF_4 are also applied in power breakers, and the importance of UF_6 in radiochemistry and nuclear technology is well known. Such thermophysical data can be used as input for numerical simulations when a cheaper and safer technology or better design are looked for. Unfortunately, accurate and systematic measurements of the thermophysical properties of these rather aggressive and toxic gaseous halides and hydrocarbons are sometimes dangerous and expensive, particularly at high temperatures. The alternative is to calculate their thermophysical properties by means of reliable intermolecular interaction potentials. A precise knowledge of these binary intermolecular potentials is also requested for the interpretation of dielectric¹ and refractivity² virial coefficients, collision-induced light scattering (CILS) spectra³ and calculation of the structure and spectroscopic properties of small clusters.⁴ All this stimulates theoretical investigations and a proper modeling of intermolecular interactions as a background for approximation of available experimental data and prediction of different transport and equilibrium properties. Moreover, if the introduced approach supplies adequate approximations of some well examined molecules like SF_6 or CF_4 , it can be applied with much more confidence to predict the properties of those gases which are scarcely measured, such as SiCl_4 , SiF_4 , etc.⁵

The main problem with the heavy globular molecules (HGMs) is that it is impossible to fit simultaneously their equilibrium and transport properties by means of only one simple spherically symmetric potential. This has been perfectly done for the noble gases and light globular molecules, such as CH_4 . The common way to deal with this problem is to look for a single effective isotropic intermolecular potential with invariable parameters producing good fit with either measured second virial coefficient $B(T)$ or viscosity $\eta(T)$. Most of the researchers fit the experimental data with the aid of an ($\exp-6$) or ($n-6$) potential, choosing convenient potential well depth ε and separation r_m . This approach explains the existence of a big variety of different $\varepsilon-r_m$ pairs for one specific molecule extracted from different experi-

ments (see, e.g., the review given by Aziz *et al.*⁶ for SF₆). In the 1970s the Heidelberg group^{7,8} has tried to fit simultaneously both transport and equilibrium properties of quasi-symmetric molecules and have reported a repulsive parameter *n* higher than 12 for some of them (SF₆, UF₆, MoF₆, WF₆). In some cases calculations for octahedral hexafluorides^{9,10} have taken into account hexadecapole moments which lead to anisotropic potentials. Unfortunately, predicted values of the hexadecapole moment are not supported by measurements in order to strengthen the evaluation of this idea.

An important step in the development of adequate models was taken further by Aziz *et al.*⁶ who achieved the best results for fitting both *B* and η of SF₆ by means of a Morse–Morse–Spline–van der Waals (MMSV) potential. This model used accurate values of the dispersion-interaction energy constant *C*₆ obtained by Kumar *et al.*¹¹ to fix the long-range contribution to the intermolecular interaction potential. However, the lack of precise *C*₆ values for other heavy globular molecules restricts its application.

In 1992 Stefanov¹² proposed a different approach to this problem which is applicable to all HGM without any preliminary assumptions for a particular molecule. He has considered the role of the vibrational excitation in the interaction between heavy globular molecules. As it is well known,^{13–15} the normal vibrational frequencies of the halides are low and a significant part of molecules is already vibrationally excited at relatively low temperatures (300–500 K). Consequently, the effective size of vibrationally excited molecules increases. Thus the concept of interactions between pairs of molecules in different vibrational modes with temperature-dependent relative populations $x_i(T)$ enables us to replace the single intermolecular potential by a set of potentials with slightly different ϵ and *r*_m. The suitability of this model has been demonstrated in the case of CF₄. A set of 55 different isotropic potentials has been used to reproduce simultaneously the experimental *B* and η data within their relative experimental error in the whole observed temperature range. Using the same vibrationally excited states of molecules (VESM) model, Stefanov and Zarkova obtained a semi-empirical intermolecular interaction potential for SF₆.^{16,17}

In this model the potential parameters are adjusted by solving an inverse ill-posed problem of minimizing the deviations between experiments and calculations (Tichonov and Arsenin¹⁸). For this determination one only needs a set of experimental *B* and η data and the normal vibrational frequencies of the considered molecule. The temperature dependence of the partial relative populations $x_i(T)$ of the vibrationally excited states are calculated via the vibrational partition function *Z*(*T*). The physical picture of the so presented interactions is equal to an increase of *r*_m and decrease of ϵ with increasing temperature. The same behavior of the potential parameters was observed by Meinander³ in his analysis of the temperature dependence of CILS spectra of SF₆. Recently, temperature-dependent intermolecular potential parameters have also been considered by Bernstein and Oref in their molecular-dynamics calculations.¹⁹ It is note-

worthy that Hoogeveen *et al.*²⁰ also obtained a change in the potential parameters with vibrational excitation for CH₃F. However, their analysis leads to a decrease of *r*_m and an increase of ϵ with the occupation of higher vibrational states. This prediction is opposite to the other observations.

The thermophysical properties of any quasispherically symmetric molecule can be calculated with the aid of the VESM model. However, the number of required potentials increases proportionally to $n_s(n_s+1)/2$. *n*_s is the number of vibrationally excited states required for the convergence of the partition function *Z*(*T*) in order to achieve good approximation. Therefore, the VESM model requires rather complicated and computationally expensive calculations, particularly for heavier molecules since *n*_s rapidly increases with the molecular weight.

It is also difficult to use this procedure for reproducing other properties related to the intermolecular potential. A criticism has been focused on the use of mixing rules to calculate η . In the recent years all these disadvantages of the VESM model were circumvented by introducing an isotropic temperature-dependent potential (ITDP) by Zarkova.²¹ This modification of the VESM approach associates the simplicity and elegance of the traditional spherically symmetric potentials with the physically adequate idea of introducing temperature-dependent *r*_m and ϵ . It can be applied to any pure globular gas as well as to binary mixtures containing at least one heavy globular gas.

In this work we present tables with recommended data for viscosity (η), second virial coefficient (*B*), and self-diffusion (ρD) of 11 polyatomic heavy globular gases, which are obtained by means of the ITDP. The paper uses already reported results of the authors and coauthors [BF₃,²² CF₄,²¹ CCl₄,⁵ SiCl₄,⁵ SiF₄,⁵ SF₆,^{16,17,21} UF₆,²³ WF₆,^{24,25} MoF₆,^{24,25} C(CH₃)₄,^{26,27} and Si(CH₃)₄^{26,27}]. A detailed analysis is presented for SF₆ because this molecule is the most investigated HGM. The multitude of available experimental data permits statistical analysis. The results can be compared with already published reference data.^{28,29} Tables of thermophysical properties for the other ten gases supply systematic information in a temperature range of 200–900 K.

The potentials of the less investigated tetrafluorides are defined following the same procedure. However, in this case tables with recommended data⁵ should be used as a first approximation in the range of extrapolation. In the case of SiCl₄ there are no available experimental *B* data. We have no choice but to put into our procedure the calculated *B*(*T*) given by Glushko³⁰ with an arbitrary relative error (of about 4%) equal to that estimated for CCl₄. This approach was motivated by a comparative analysis of the results for the quite similar tetrahedral molecules CF₄, CCl₄, and SiF₄. Thus, the tables for SiCl₄ must be accepted critically.

The algorithms and tables for $r_m^{(\text{eff})}(T)$, $\epsilon^{(\text{eff})}(T)$, and the repulsive parameter *n* given for all gases can be used to calculate potential-dependent properties in a wide temperature range. In addition, we also present polynomial fits of *B*,

η , and self-diffusion ρD as a function of temperature.

2. Isotropic Temperature-Dependent Potential (ITDP)

The ITDP approach²¹ is a rationalized version of the model of the VESM proposed in 1992 by Stefanov.¹² It was introduced in order to speed up the calculations for heavy molecules (UF_6 ,²³ WF_6 ,^{23,24} MoF_6 ^{23,24}) and mixtures of different globular molecules.³¹ It permits us to obviate some theoretical difficulties bound to the calculation of the viscosity of the considered globular gas as a mixture of different vibrationally excited states.¹² As it can be seen for, e.g., UF_6 ,²³ for temperatures $T > 300$ K practically all molecules are already excited and the number of states which ensures the convergence of the partition function is large ($n_s \approx 200\,000$). Moreover, it is impossible to find even a small group of excited states which remain populated enough in the whole temperature range. These problems make the use of the VESM model inadequate because of the enormously increasing computational time [proportional to $\frac{1}{2}n_s(n_s+1)$].

The ITDP has been discussed in detail elsewhere (see, for example, Zarkova *et al.*^{21,23,26}). It will be outlined here briefly.

Instead of a mixture of n_s different vibrational states,¹² we now consider the globular gas at given temperature T to consist only of one vibrationally excited state with an enlargement of the molecular radii $\delta^{(\text{eff})}(T)$ averaged over all n_s states:

$$\delta^{(\text{eff})} = \sum_{l,m=0}^{n_s} \delta(T=0) \times [C_l \times x_l(T) + C_m \times x_m(T)]. \quad (1)$$

The harmonic oscillator force constants, $C_{l,m}$, are known and equal to the enlargement of the excited level k ($k=l,m$) normalized to the enlargement $\delta(T=0)$ of the first level.²³ x_k ($k=l,m$) is the relative population of the excited state k ($\sum_{k=0}^{n_s} x_k(T) = 1$). It is calculated as a function of temperature by means of the vibrational partition function

$$Z(T) = 1 + \sum_{n=1}^{\infty} \sum_{v_i=0}^n \dots \sum_{v_N=0}^{n-v_1-\dots-v_{N-1}} \prod_{i=1}^N g_{v_i} \times \exp(-v_i \theta_i/T), \quad (2)$$

where N is the total number of normal vibrations, v_i is the quantum number of the vibrationally excited level of i th normal vibration, and g_{v_i} is the degeneracy; $\theta_i = h v_i / k$, where v_i is the i th normal vibrational frequency. The relative population of the ground state is $x_0 = 1/Z$.

The interactions between excited molecules with an averaged effective size at given T can be described by means of a single isotropic ($n-m$) or ($n-\text{exp}$) potential, respectively. If the ($n-6$) model is chosen then the effective potential $U(r,T)$ is

$$U(r,T) = \frac{\varepsilon^{(\text{eff})}}{n-6} \left\{ 6 \left[\frac{r_m^{(\text{eff})}}{r} \right]^n - n \left[\frac{r_m^{(\text{eff})}}{r} \right]^6 \right\}, \quad (3)$$

where r is the distance between the centers of mass of the two molecules and n is the repulsive parameter.

In Eq. (3) the effective equilibrium distance is

$$r_m^{(\text{eff})}(T) = r_m + \delta^{(\text{eff})}(T) \quad (4)$$

and the effective potential depth well is

$$\varepsilon^{(\text{eff})} = \varepsilon \left[\frac{r_m}{r_m^{(\text{eff})}} \right]^6. \quad (5)$$

Relation (5) follows from the assumption that the long-range forces are not influenced by excitation.

In both equations (4) and (5) $r_m = r_m(T=0)$ and $\varepsilon = \varepsilon(T=0)$ are parameters of the ground state-ground state interaction. It is obvious that the temperature dependence of $r_m^{(\text{eff})}$ is implied in the dependence $C_k x_k(T)$, which is specific for a particular globular gas. It can be calculated accurately by means of Eq. (2) and then approximated with a high precision. Subsequently this relation can be used to calculate $\varepsilon^{(\text{eff})}$ by using Eq. (5).

We consider separately the behavior of the potential [Eq. (3)] at short and long ranges in order to justify the choice of the shape of $U(r)$.

(a) *Short-range part of the potential.* Both ($n-6$) and ($\text{exp}-6$) potentials may approximate equally well the measured values of viscosity and of the second virial coefficient. Theoretically the short-range forces are described by exponentials. In our experience with mercury³² we found that within a very good accuracy ($n-6$) and ($\text{exp}-6$) coincide.

(b) *The long-range part of the potentials* in our model is unaffected by the vibrational excitation. This assumption is not valid at very high temperatures, which are not considered here.

3. Experimental Data

In general, the determination of the ITDP parameters is based on the experimental pVT -second virial coefficients B and viscosity η . Acoustic second virial coefficients β are available only for tetramethyl methane.³³ In this case they were also included into the minimization procedure.

The input sets of experimental data were critically analyzed. Those of them which were not consistent with the majority of the other data or which contradict theory were excluded from the minimization procedure. To this end a so-called "jack-knife control"³⁴ was applied. This procedure allowed us to analyze the consistency of each experimental data set with the basic data set. It gave an objective reason to accept or to reject a specific work no matter what accuracy the authors claim. For instance, owing to this procedure, we rejected the viscosity data for SF_6 of Lukin *et al.*^{35,36} A careful analysis confirmed our conclusion and showed that a similar discrepancy between these data and standard data was observed also in the case of the viscosity of noble gases. As a rule, when there were enough experimental data we did not use those data which are derived from the measurements by means of models with unknown input parameters [e.g., $B(T)$ derived from special refractivity measurements].

In the following tables with experimental data used in our minimization are presented (Tables 1–11). In all cases, M is the number of experimental data, ΔT the temperature range in K, and a_{exp} the relative experimental error in percent. The normal vibrational frequencies used for the calculation of the partition function $Z(T)$ are given in Tables 12 and 13 (see Sec. 6).

3.1. Planar Heavy Globular Molecules (BF_3)

TABLE 1. BF_3 . Set of experimental data used for approximation

Reference	Property	M	$\Delta T/\text{K}$	$a_{\text{exp}}/\text{percent}$
1. Raw ³⁷ (1961)	B	5	293–343	5.1–8.1
2. Viswanath ³⁸ (1966)	B	7	273–333	5
3. Waxman <i>et al.</i> ³⁹ (1973)	B	13	273–498	10
4. Cooke and McKenzie ⁴⁰ (1951)	η	5	306–459	3
5. McCoubrey and Singh ⁴¹ (1957)	η	6	292–453	2
6. Ellis and Raw ⁴² (1959)	η	4	453–623	2
7. Menabde ⁴³ (1968)	η	14	173–293	1
8. Ho ⁴⁴ (1988)	η	5	200–600	3
all B data	B	25	273–498	
all η data	η	34	173–623	
all B and η data	$B + \eta$	59	173–623	

3.2. Tetrahedral Heavy Globular Molecules (CF_4 , SiF_4 , CCl_4 , SiCl_4)

The fluorine and chlorine containing HGM are among the most widespread gases in contemporary chemical and electrical engineering.⁴⁵ Unfortunately, CF_4 is the only tetrahedral HGM, which can be considered as well examined. There are considerably less data for CCl_4 and SiF_4 . In the case of SiCl_4 very little information is available.

In an earlier work⁵ we suggested an approach to the calculation of self-consistent thermophysical properties of scarcely examined tetrahedral molecules. It was used to predict B , η and ρD for SiF_4 and SiCl_4 in a temperature range exceeding that of the available experiments. In the case of the ITDP the temperature dependence of r_m and ε is attributed to the change of the relative populations of the vibrationally excited molecules.³¹ If the normal vibrational frequencies are known, $x_k(T)$ can be defined via $Z(T)$ without additional experimental data. This allows us to predict the ITDP parameters of molecules with insufficiently measured thermophysical properties. In these cases we have no other choice but to use in the minimization procedure all known primary and secondary (calculated or estimated) data as well as the unpublished values of second virial coefficients $B(T)$ for SiF_4 ^{46,47} cited by Dymond and Smith.⁴⁸ In all following tables such data will be marked with an asterisk.

3.2.1. Carbon tetrafluoride, CF_4

In our first representation of the ITDP²¹ we used the same 84 experimental points (ten experiments) that were considered earlier by Stefanov¹² and obtained the same potential parameters (PPs). The selection of the experimental set has limited the temperatures up to 500 K. Applying a new computational routine to consider all existing vibrationally ex-

TABLE 2. CF_4 . Set of experimental data used for approximation

Reference	Property	M	$\Delta T/\text{K}$	$a_{\text{exp}}/\text{percent}$
1. Cawood and Patterson ⁵⁰ (1937)	B	1	294	10
2. McCormac and Schneider ⁵¹ (1951)	B	7	273–673	10
3. Hamann <i>et al.</i> ⁵² (1954)	B	5	313–398	1
4. Douslin <i>et al.</i> ⁵³ (1961)	B	16	273–623	1–8
5. Kalfoglu and Miller ⁵⁴ (1967)	B	6	303–773	3
6. Lange Jr. And Stein ⁵⁵ (1970)	B	6	203–369	3
7. Sigmund <i>et al.</i> ⁵⁶ (1972)	B	6	271–423	1–3
8. Bose <i>et al.</i> ⁵⁷ (1972)	B	3	279–373	3
9. Utenskov ⁵⁸ (1976)	B	16	173–323	2–3
10. Schramm and Müller ⁵⁹ (1982)	B	1	296	2
11. Elias <i>et al.</i> ⁶⁰ (1986)	B	3	173–203	3.5
12. Boyes <i>et al.</i> ⁶¹ (1990)	B	9	175–375	2
13. Bignell and Dunlop ⁶² (1993)	B	3	290–310	10
14. Schramm <i>et al.</i> ^{49*} (2000)	B	11	203–773	0.13–5
15. McCubrey and Singh ⁴¹ (1957)	η	10	314–455	1
16. Dawe <i>et al.</i> ⁶³ (1970)	η	19	293–823	0.5
17. Genot ⁶⁴ (1970)	η	16	296–673	11.5
18. Hellmanns <i>et al.</i> ⁶⁵ (1973)	η	9	298–873	0.5
19. Kestin <i>et al.</i> ⁶⁶ (1977)	η	9	245–346	1
all B	B	93	173–773	
all η	η	63	173–873	
all $B + \eta$	$B + \eta$	156	173–873	

cited states at given T , we were able to extend the experimental data set which now consists of 156 experimental points (19 experiments) measured in the range between 175 and 873 K.

Recently Schramm *et al.*⁴⁹ have published $B(T)$ estimated on the background of their new measurements. Given the high temperature range (203–773 K) and the high accuracy of estimation, these data convinced us once more in the reliability of the adjustment of the ITDP parameters.

3.2.2. Silicon tetrafluoride, SiF_4

TABLE 3. SiF_4 . Set of experimental data used for approximation

Reference	Property	M	$\Delta T/\text{K}$	$a_{\text{exp}}/\text{percent}$
1. Hamann <i>et al.</i> ⁶⁷ (1953)	B	8	293–353	4
2. Schramm and Schmiedel ⁴⁶ (1979)	B	7	295–475	10
3. Schramm and Gehrmann ⁴⁷ (1979)	B	6	205–295	6
4. McCubrey and Singh ⁴¹ (1957)	η	14	291–464	2
5. Ellis and Raw ⁴² (1959)	η	15	296–607	3
6. Li <i>et al.</i> ⁶⁸ (1978)	η	5	313–473	3
all B data	B	21	205–475	
all η data	η	46	291–607	
all B and η data	$B + \eta$	67	205–607	

3.2.3. Carbon tetrachloride, CCl_4

The carbon tetrachloride has not been recently investigated. To obtain more reliable potential parameters within the frame of the restricted number of available measurements, we discarded three of the obviously inaccurate experimental points of Lambert *et al.*⁶⁹ The self-consistency of the

TABLE 4. CCl_4 . Set of experimental data used for approximation

Reference	Property	M	$\Delta T/\text{K}$	$a_{\exp}/$ percent
1. Lambert <i>et al.</i> ⁶⁹ (1949)	B	10	319–351	4
2. Francis and McGlashan ⁷⁰ (1955)	B	5	316–343	4
3. Perez Masia <i>et al.</i> ⁷¹ (1963)	B	4	353–419	4
4. Braune and Linke ⁷² (1930)	η	9	296–761	3
5. Sperry and Mack Jr. ⁷³ (1932)	η	5	323–523	1.5
6. Titani ⁷⁴ (1933)	η	6	401–588	3
7. Mueller and Ignattowski ⁷⁵ (1960)	η	3	293–413	0.7–3.3
8. Lapidus <i>et al.</i> ^{76*} (1968)	η	10	273–573	3
9. Vargaftic ^{77*} (1975)	η	7	273–873	3
10. Lucas ⁷⁸ (1987)	η	3	398–573	3
all B data	B	19	316–419	
all η data	η	43	273–761	
all B and η data	$B + \eta$	62	273–761	

solution was confirmed by the covariance–variance matrix. Further on, the approximation of $B(T)$ given by Dymond and Smith⁴⁸ was used for a verification.

3.2.4. Silicon tetrachloride, SiCl_4

TABLE 5. SiCl_4 . Set of experimental data used for approximation

Reference	Property	M	$\Delta T/\text{K}$	$a_{\exp}/$ percent
1. Gloushko ^{30*} (1979)	B	21	400–800	8
2. Lel'chuk and Tubianskaia ⁷⁹ (1961)	η	2	273–330	1.5
3. Drew <i>et al.</i> ^{45*} (1973)	η	8	273–973	5
4. Lapidus <i>et al.</i> ^{76*} (1968)	η	10	273–573	3
all B data	B	21	40–800	
all η data	η	20	273–973	
all B and η data	$B + \eta$	41	273–973	

3.3. Octahedral Heavy Globular Molecules (SF_6 , MoF_6 , WF_6 , UF_6)

The experimental data for the hexafluoride gases (with the exception of SF_6) are not compatible and sometimes it is difficult to judge their quality and accuracy. Therefore, we choose to consider all of them taking the risk that the results will be somewhat approximate.

TABLE 6. SF_6 . Set of experimental data used for approximation

Reference	Property	M	$\Delta T/\text{K}$	$a_{\exp}/$ percent
1. MacCormac and Schneider ⁵¹ (1951)	B	5	273–523	3–10
2. Hamann <i>et al.</i> ⁶⁷ (1953)	B	16	293–448	2–5
3. Clegg <i>et al.</i> ⁸¹ (1955)	B	5	307–404	3–4
4. Jerdev ⁸² (1970)	B	11	253–473	6
5. Hajjar and MacWood ⁸³ (1970)	B	2	343–373	3–3.5
6. Sigmund <i>et al.</i> ⁵⁶ (1972)	B	7	271–423	1–3
7. Hosticka and Bose ⁸⁴ (1974)	B	3	323–374	7
8. Bellm <i>et al.</i> ⁸⁵ (1974)	B	10	300–550	1.5–8.5
9. Hahn <i>et al.</i> ⁸⁶ (1974)	B	9	200–472	7
10. Timoshenko <i>et al.</i> ⁸⁷ (1976)	B	6	313–413	2–4
11. Santafe <i>et al.</i> ⁸⁸ (1976)	B	6	273–323	1.2–4
12. St-Arnaud and Bose ⁸⁹ (1979)	B	1	323	5
13. Biswas <i>et al.</i> ⁹⁰ (1984)	B	1	333	3
14. Molerup ⁹¹ (1985)	B	4	260–340	1.2–2
15. Elias <i>et al.</i> ⁶⁰ (1986)	B	1	296	3.5
16. McCubrey and Singh ⁴¹ (1957)	η	8	295–478	2
17. Ellis and Raw ⁴² (1959)	η	11	470–973	3
18. Dawe <i>et al.</i> ⁶³ (1970)	η	18	293–873	1
19. Kestin <i>et al.</i> ⁹² (1971)	η	2	296–302	0.5
20. Hellemans <i>et al.</i> ⁶⁵ (1973)	η	7	298–573	0.6
21. Veda and Kigoshi ⁹³ (1974)	η	8	273–346	1
22. Timrot <i>et al.</i> ⁹⁴ (1975)	η	8	299–523	0.5
23. Kestin <i>et al.</i> ⁹⁵ (1976)	η	3	296–477	0.5
24. Kestin <i>et al.</i> ⁶⁶ (1977)	η	5	298–473	0.5
25. Kestin <i>et al.</i> ⁶⁶ (1977)	η	7	297–473	0.5
26. Abe <i>et al.</i> ⁹⁷ (1979)	η	2	423–468	0.5
27. Harris <i>et al.</i> ⁹⁸ (1979)	η	7	218–302	0.7–1.5
28. Tanaka <i>et al.</i> ⁹⁹ (1980)	η	3	298–348	2
29. Hoogland <i>et al.</i> ¹⁰⁰ (1985)	η	5	298–333	0.5
30. Strehlow and Vogel ⁸⁰ (1989)	η	9	298–673	0.2–0.3
all B data	B	87	199–550	
all η data	η	103	218–973	
all $B + \eta$ data	$B + \eta$	190	199–973	

3.3.1. Sulfur hexafluoride, SF_6

Altogether 190 experimental points of B and η from 30 works listed in Table 6 were used to determine the ITDP parameters in the temperature range between 200 and 970 K. Compared to our previous paper²¹ new and more accurate results of the viscosity⁸⁰ were used and a new computational code was built up for rigorous calculations of the whole set of vibrationally excited states. As a result the potential parameters were adjusted more precisely although the changes are not substantial.

3.3.2. Molybdenum hexafluoride, MoF_6

TABLE 7. MoF_6 . Set of experimental data used for approximation

Reference	Property	<i>M</i>	$\Delta T/\text{K}$	$a_{\exp}/\text{percent}$
1. Malishev ¹⁰¹ (1974)	<i>B</i>	25	300–593	3.5–5
2. Morizot <i>et al.</i> ¹⁰² (1973)	<i>B</i>	8	313–453	5
3. Heintz and Lichtenhaler ⁸ (1976)	<i>B</i>	15	320–460	3
4. Osborne <i>et al.</i> ¹⁰³ (1966)	<i>B</i>	2	298.15	3.5
5. Morizot <i>et al.</i> ¹⁰⁴ (1973)	η	6	313–413	5
all <i>B</i> data	<i>B</i>	49	298–593	
all η data	η	6	313–413	
all <i>B</i> and η data	<i>B</i> + η	55	298–593	

3.3.3 Tungsten hexafluoride, WF_6

TABLE 8. WF_6 . Set of experimental data used for approximation

Reference	Property	<i>M</i>	$\Delta T/\text{K}$	$a_{\exp}/\text{percent}$
1. Malishev ¹⁰¹ (1974)	<i>B</i>	28	281–592	3–5
2. Morizot <i>et al.</i> ¹⁰² (1973)	<i>B</i>	8	313–453	5
3. Heintz and Lichtenhaler ⁸ (1976)	<i>B</i>	16	320–462	3
4. Morizot <i>et al.</i> ¹⁰⁴ (1973)	η	7	313–433	5
all <i>B</i> data	<i>B</i>	52	281–592	
all η data	η	7	313–433	
all <i>B</i> and η data	<i>B</i> + η	59	281–592	

3.3.4 Uranium hexafluoride, UF_6

TABLE 9. UF_6 . Set of experimental data used for approximation

Reference	Property	<i>M</i>	$\Delta T/\text{K}$	$a_{\exp}/\text{percent}$
1. Magnuson ¹⁰⁵ (1955)	<i>B</i>	8	326–405	2.5–9
2. Malyshev ¹⁰⁶ (1972)	<i>B</i>	15	463–592	4
3. Malyshev ¹⁰⁷ (1973)	<i>B</i>	6	320–370	4
4. Morizot <i>et al.</i> ¹⁰² (1973)	<i>B</i>	9	328–463	10
5. Heintz <i>et al.</i> ⁷ (1976)	<i>B</i>	19	320–469	1.9–4
6. Kigoshi ¹⁰⁸ (1950)	η	4	287–318	
7. Llewellyn ¹⁰⁹ (1953)	η	6	273–473	
8. Morizot <i>et al.</i> ¹⁰⁴ (1973)	η	7	328–433	
9. Myerson and Eicher ¹¹⁰ (1952)	η	7	313–473	
all <i>B</i> data		57	273–592	
all η data		24	273–473	
all <i>B</i> and η data		81	273–592	

3.4. Tetramethyl Compounds $\text{C}(\text{CH}_3)_4$, $\text{Si}(\text{CH}_3)_4$

Following in general the same procedure that has been applied to the tetrahedral and octahedral molecules, for this kind of HGM we met some more complicated problems. The calculation of the vibrational partition function of complex molecules consisting of many atoms might be a problem because of the lack of a full set of accurate normal vibrational frequencies. For XY_4Z_{12} molecules their number is $N=3l-6=45$ (*l* being the number of atoms), and only a part of them were known. The problem has been successfully resolved by means of convenient experimental and mathematical methods (see our recently published papers).^{26,27}

3.4.1 Tetramethyl Methane, $\text{C}(\text{CH}_3)_4$

TABLE 10. $\text{C}(\text{CH}_3)_4$. Set of experimental data used for approximation

Reference	Property	<i>M</i>	$\Delta T/\text{K}$	$a_{\exp}/\text{percent}$
1. Beattie <i>et al.</i> ¹¹¹ (1952)	<i>B</i>	6	434–548	10
2. Hamann <i>et al.</i> ¹¹² (1955)	<i>B</i>	11	303–403	10
3. Heichelheim and McKetta ¹¹³ (1963)	<i>B</i>	9	303–473	1.2–3
4. Perez Masia <i>et al.</i> ⁷¹ (1963)	<i>B</i>	5	303–398	1.6–3
5. Silberberg <i>et al.</i> ¹¹⁴ (1967)	<i>B</i>	9	303–473	2
6. Dawson <i>et al.</i> ¹¹⁵ (1973)	<i>B</i>	9	348–498	0.8–1.5
7. Das <i>et al.</i> ¹¹⁶ (1977)	<i>B</i>	14	303–548	5
8. Ewing and Marsh ¹¹⁷ (1979)	<i>B</i>	3	303–346	0.5–0.8
9. Hossenlopp and Scott ¹¹⁸ (1981)	<i>B</i>	8	265–304	1–2.6
10. Ewing <i>et al.</i> ³³ (1987)	β	8	250–323	1
11. McCubrey ¹¹⁹ (1960)	η	4	351–456	1
12. Gonzales and Lee ¹²⁰ (1968)	η	5	310–444	1
13. Diaz Pena and Esteban ¹²¹ (1966)	η	16	263–393	1
14. Lambert <i>et al.</i> ¹²² (1955)	η	4	323–351	1
all <i>B</i> data		74	265–548	
all η data		29	263–458	
all β data		8	250–323	
all <i>B</i> , η and β data		111	250–548	

3.4.2 Tetramethyl Silane, $\text{Si}(\text{CH}_3)_4$

TABLE 11. $\text{Si}(\text{CH}_3)_4$. Set of experimental data used for approximation

Reference	Property	<i>M</i>	$\Delta T/\text{K}$	$a_{\exp}/\text{percent}$
1. Hamann <i>et al.</i> ¹¹² (1955)	<i>B</i>	6	323–403	10
2. Bottomley and Nairn ¹²³ (1977)	<i>B</i>	13	294–539	0.5–2.2
3. Marcos <i>et al.</i> ¹²⁴ (1983)	<i>B</i>	7	423–572	10
4. Diaz Pena and Esteban ¹²¹ (1966)	η	17	263–413	1
all <i>B</i> data	<i>B</i>	26	323–572	
all η data	η	17	263–413	
all <i>B</i> and η data	<i>B</i> + η	43	263–572	

TABLE 12. Normal vibrational frequencies and degeneracies (in parentheses) used in calculations: planar, tetrahedral, and octahedral molecules

	BF_3^{a}	CF_4	SiF_4	CCl_4	SiCl_4	SF_6	MoF_6	WF_6	UF_6
ν_1/cm^{-1}	887.6 (1)	908.2 (1)	801.0 (1)	459.0 (1)	424.0(1)	770.0(1)	741.0(1)	769.0(1)	667.0(1)
ν_2/cm^{-1}	696.2 (1)	434.5 (2)	264.0(2)	218.0(2)	150.0(2)	640.0(2)	326.0(2)	670.0(2)	543.1(2)
ν_3/cm^{-1}	1469.6 (2)	1272.0 (3)	111.4.(3)	776.0(3)	608.0(3)	522.0(3)	741.0(3)	712.0(3)	626.1(3)
ν_4/cm^{-1}	480.6 (2)	632 (3)	386.35(3)	312.0(3)	224.0(3)	345.0(3)	262.0(3)	256.0(3)	186.1(3)
ν_5/cm^{-1}						615.0(3)	312.0(3)	322.0(3)	200.1(3)
ν_6/cm^{-1}						947.0(3)	122.0(3)	216.0(3)	143.2(3)

^aReferences are: BF_3 : Pak and Woods;¹³⁰ CF_4 , CCl_4 , SIF_4 , SiCl_4 , and SF_6 : Krasnov;¹³¹ UF_6 : McDowell *et al.*;¹³² WF_6 : McDowell *et al.*;¹³³ MoF_6 : Glassen *et al.*¹³⁴

4. Methodology

4.1. SF_6 as an Example

Gaseous SF_6 is a reasonable candidate to demonstrate the quality of the ITDP. Due to the wide practical interest in this gas it is probably the most experimentally and theoretically investigated heavy quasispherical molecule. The large number of experimental data which depend essentially on the intermolecular interaction potential allows us to prove the reliability of our approach by means of different statistical tests. The quality of the produced data for B and η is certified by a comparison with other available models (see, for example, Aziz *et al.*⁶ and with tabulated properties which are obtained in a wide range of temperature (see Boushehri *et al.*²⁸ and Trengove and Wakeham.²⁹

4.1.1. Best Solution and Deviation Plots

The ITDP parameters are determined by solving a typical “ill-posed” problem¹⁸ of minimizing the sum of squared deviations $F = \sum_M (R_i^2) = \sum_M [\ln(P_{i,\text{exp}}/P_{i,\text{calc}})/a_{i,\text{exp}}]^2$ between M measured (P_{exp}) and calculated (P_{calc}) values of B and η normalized to their relative experimental error a_{exp} . It is noteworthy that the only input data required for obtaining the ITDP for any particular HGM are the normal vibrational frequencies and as much as possible experimental data of different kind. In the case of SF_6 we have used data of the second pVT -virial coefficient $B(T)$ and of the viscosity $\eta(T)$ as input data. All these values and in addition the acoustic second virial coefficients as well are calculated by means of the well known formulas for pure gases.¹⁴ The root mean square deviations $\text{RMS} = \sqrt{F/M}$ and the mean relative deviations $\langle R \rangle = M^{-1} \sum_M \ln(P_{i,\text{exp}}/P_{i,\text{calc}})/a_{i,\text{exp}}$ are normalized to $a_{i,\text{exp}}$.

The parameters of the best fitting potential for SF_6 ($\text{RMS} = 0.657a_{\text{exp}}$) obtained in this way are: potential well depth $\varepsilon = 417.80(87)$ K, equilibrium distance $r_m = 5.041(3) \times 10^{-10}$ m, repulsive parameter $n = 34.76(33)$, and first level enlargement $\delta = 1.31(3) \times 10^{-12}$ m.

The distribution of the mean RMS deviations and mean absolute deviations in Table 14 do not show any systematic deviation in the whole temperature range of measurements (200–973 K). The weighted relative deviations R_{iB} and $R_{i\eta}$ obtained with these parameters are plotted in Fig. 1. The most part of them (about 90%) are in the frame of $\pm 1 a_{\text{exp}}$. In the whole temperature range the deviations are situated

symmetrically with respect to the reference line, which is given by our solution. The mean relative deviations in units of the accepted experimental errors are $\langle R_{iB} \rangle = -0.045a_{\text{exp}}$ (for B only $\text{RMS} = 0.570a_{\text{exp}}$) and $\langle R_{i\eta} \rangle = -0.182a_{\text{exp}}$ (for η only $\text{RMS} = 0.676a_{\text{exp}}$).

In order to check the sensitivity of our solution to the variations of the PP, we successively changed one of them (for example, n) while the other three (in that case ε , r_m and δ) were kept fixed. Subsequently, the obtained $\text{RMS}_{\text{fixed}}$ were compared with that of the “best” solution ($\text{RMS} = 0.657a_{\text{exp}}$). The normalized deviations ($\text{RMS}_{\text{fixed}}/\text{RMS}$) as functions of the change of the potential parameters ($\pm \Delta \text{PP}$ in percent) are shown in Table 15. The results convince us that the choice of all parameters is reliable: $\text{RMS}_{\text{fixed}}$ increases when each of the parameters has been changed in both (\pm) directions. The influence of δ and n is relatively weak. Changing each of them by $\pm 3\%$ practically does not affect the solution. In the case of changing δ we obtain $\text{RMS}_{\text{fixed}} = 1.03 \text{ RMS}$ and in the case of changing n $\text{RMS}_{\text{fixed}} = 1.18 \text{ RMS}$ results. The solution is much more sensitive to a change in the potential well depth ε ($\text{RMS}_{\text{fixed}} = 3.4 \text{ RMS}$ for

TABLE 13. Normal vibrational frequencies and degeneracies (in parentheses) used in calculations: tetramethyl compounds

No	Mode	Frequencies, (cm^{-1}) ^a	
		$\text{C}(\text{CH}_3)_4$	$\text{Si}(\text{CH}_3)_4$
1	A2	239	153
2	T1	308	157
3	E	335	180
4	T2	415	223
5	A1	733	573
6	T2	921	683
7	T1	953	690
8	E	1075	827
9	T2	1249	879
10	T2	1365	1264
11	A1	1400	1270
12	T1	1444	1417
13	E	1451	1419
14	T2	1477	1433
15	T2	2863	2888
16	A1	2909	2891
17	T1	2954	2960
18	E	2955	2961
19	T2	2959	2964

^aData taken from Zarkova *et al.*²⁶

TABLE 14. The distribution of the RMS and $\langle R_i \rangle$ deviations of SF₆ as a function of temperature

Second virial coefficient				Viscosity			
ΔT (K)	M	$\langle R_{iB} \rangle$ (a_{exp})	RMS (B) (a_{exp})	ΔT (K)	M	$\langle R_{i\eta} \rangle$ (a_{exp})	RMS (η) (a_{exp})
199–300	18	−0.327	0.587	200–300	21	0.218	0.703
301–350	33	0.032	0.659	301–400	34	−0.305	0.720
351–400	17	0.210	0.509	401–500	22	−0.289	0.689
401–450	11	0.038	0.438	501–700	15	0.011	0.684
451–550	8	−0.393	0.574	700–1000	11	−0.624	0.785
199–550	87	−0.045	0.571	200–1000	103	−0.182	0.676

$\Delta\varepsilon = \pm 3\%$). The strongest variation is observed in the case of r_m , where a variation of $\Delta r_m = \pm 3\%$ leads to a 20-fold increase in RMS. In view of the ITDP this behavior of RMS_{fixed} is not surprising because by definition of the ITDP [see Eq. (5)] a change in r_m results in a simultaneous change of ε , too. Of course, there is enough room for further adjustments of the potential parameters when new experimental input data are available. For example, accurate measurements of the speed of sound could supply new data for the acoustic second-virial coefficient. The quality of these data as experimental input data has recently been demonstrated in the case of TMM.^{26,27}

In our model the temperature dependence of the potential parameters r_m and ε arises from the vibrational excitation. This model also allows for the inclusion of other temperature-dependent effects (for example, rotational excitation or q deformation). If these effects will be taken into account, probably a change in n and δ will occur.

The relative B and η deviations are plotted in Figs. 2 and 3, respectively. Apparently, the experimentally obtained second virial coefficients are consistent at temperatures higher than 250 K. However, the low temperature region ($T < 250$ K) is poorly reproduced. There are only three measured data points of $B(T)$ at $T < 250$ K, reported by Hahn *et al.*⁸⁶ They are reproduced with a deviation of less than 1 a_{err} which is given as 7%. At 199 K the measured value of B is $-693 \text{ cm}^3 \text{ mol}^{-1}$; our prediction of $B_{\text{calc}} = -655.35 \text{ cm}^3 \text{ mol}^{-1}$ practically coincides with that reported by Aziz *et al.*⁶ ($-646.6 \text{ cm}^3 \text{ mol}^{-1}$).

Our calculated viscosities coincide to 1% with the most accurate measurements ($a_{\text{exp}} \leq 1\%$, see Table 6). These experimental input data have a strong influence on our solution.

A “jack-knife” procedure³⁴ was applied to the experiments in order to clarify their impact on the potential parameters (Table 16). For example, when excluding the viscosity data measured by Strehlow and Vogel⁸⁰ ($a_{\text{exp}} = 0.2\% – 0.3\%$) the largest change of the shape of the potential was observed (Table 16, row 28: $\varepsilon = 408.4 \text{ K}$, $r_m = 5.057 \times 10^{-10} \text{ m}$, $n = 32.06$, $\delta = 1.42 \times 10^{-12} \text{ m}$). This test also illustrates that our solution is an acceptable compromise between the contradictory influences of B and η on the shape of the potential (rows 29–31, Table 16).

4.1.2. Comparison with Available B and η Calculations

As a further test we compare our findings with the published reference data. Boushehri *et al.*²⁸ have presented B and η tables, whereas Trengove and Wakeham²⁹ only gave tables for the viscosity. All data are given in a wide temperature range. In both papers the authors are employing the corresponding states principle to predict viscosity²⁹ or pVT -second virial coefficient, viscosity, and diffusion²⁸ of SF₆. In the second case the (6–12) Lennard-Jones (LJ) PP are determined from viscosity. With so obtained ε and σ the authors calculate other transport properties (self-diffusion coefficient, isotropic thermal diffusion factor), as well as the spherical part of $B(T)$. The nonspherical contributions to be taken into account have to be calculated from other known molecular properties (quadrupole moments, polarizability anisotropy). Although the results for the second virial coefficients are not quite satisfying, the paper is between the first attempts to solve the problem of fitting simultaneously equilibrium and transport properties of molecular gases.

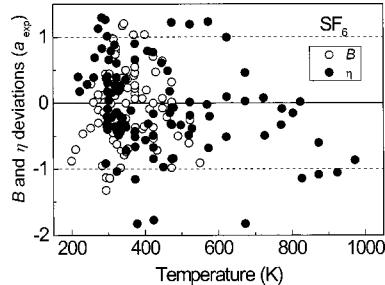


FIG. 1. Weighted relative deviations of measured $B(T)$ and $\eta(T)$ of SF₆ from the best solution obtained with the ITDP (zero line).

TABLE 15. Influence of the change of the parameters PP on the RMS(PP) deviations normalized to the “best” solution deviation (RMS = 0.657 a_{exp})

ΔPP (%)	RMS (fixed δ)/ RMS	RMS (fixed n)/ RMS	RMS (fixed ε)/ RMS	RMS (fixed r_m)/ RMS
0	1.00	1.00	1.00	1.00
1	1.00	1.02	1.47	6.60
2	1.01	1.08	2.38	13.1
3	1.03	1.18	3.39	19.7

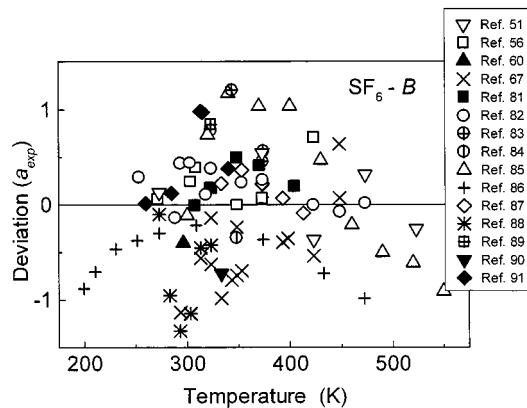


FIG. 2. Relative deviations of the second *pVT*-virial coefficient for the individual experimental input data of SF₆.

In Fig. 4 we show the absolute deviations between our calculations (reference line) and the data presented in Refs. 28 and 29 which were not used in the minimization procedure. For comparison the experimental viscosity data which are measured with an accuracy of at least 0.5% are also shown. These data have been taken into account in our minimization procedure, of course. One can notice that although

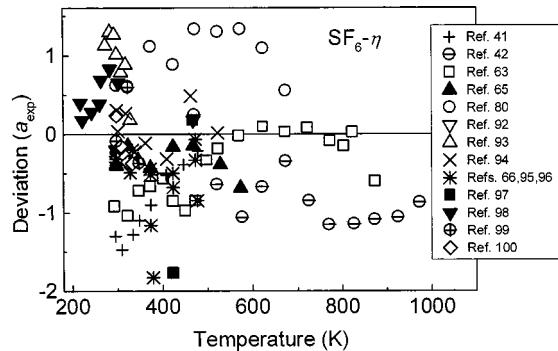


FIG. 3. Relative deviations of the viscosity for the individual experimental input data of SF₆.

the deviations are relatively small ($< \pm 1\%$ and $< \pm 0.4\%$ for Boushehri *et al.*²⁸ and Trengove and Wakeham,²⁹ respectively), at $T > 300$ K they are systematically negative. The explanation is that both papers^{28,29} appeared before the measurements of Strehlow and Vogel⁸⁰ were published. The latter data, obtained in the temperature range between 298 and 673 K, are included in our minimization procedure. It has been shown already (see Sec. 4.1.1) that they have the strongest impact on our “best” solution.

TABLE 16. The influence of the specific experimental data on our solution for SF₆ (“jack-knife” check)

No	Excluded experiment	M	ΔT (K)	ε (K)	r_m (10^{-10} m)	n	δ (10^{-12} m)	RMS a_{err}
1	MacCormac and Schneider ⁵¹ (B)	185	273–523	416.70	5.040	34.76	1.32	0.663
2	Hamann <i>et al.</i> ⁶⁷ (B)	174	293–448	415.69	5.043	34.74	1.30	0.653
3	Clegg <i>et al.</i> ⁸¹ (B)	185	307–404	416.76	5.041	34.78	1.31	0.663
4	Jerdev ⁸² (B)	179	253–473	417.33	5.041	34.78	1.31	0.673
5	Hajjar and MacWood ⁸³ (B)	188	343–373	416.80	5.041	34.78	1.31	0.653
6	Sigmund <i>et al.</i> ⁵⁶ (B)	183	271–423	417.02	5.040	34.80	1.31	0.666
7	Hosticka and Bose ⁸⁴ (B)	187	323–374	416.72	5.04	34.76	1.32	0.658
8	Belm <i>et al.</i> ⁸⁵ (B)	180	300–550	417.37	5.040	34.62	1.38	0.659
9	Hahn <i>et al.</i> ⁸⁶ (B)	181	200–472	416.30	5.042	34.66	1.33	0.658
10	Timoshenko <i>et al.</i> ⁸⁷ (B)	184	313–413	416.90	5.040	34.76	1.32	0.662
11	Santafe <i>et al.</i> ⁸⁸ (B)	184	273–323	415.57	5.043	34.75	1.27	0.647
12	St-Arnaud and Bose ⁸⁹ (B)	189	323	416.78	5.040	34.77	1.32	0.653
13	Biswas <i>et al.</i> ⁹⁰ (B)	189	333	416.63	5.041	34.76	1.32	0.656
14	Molerup ⁹¹ (B)	186	260–340	417.17	5.040	34.77	1.33	0.659
15	Elias <i>et al.</i> ⁶⁰ (B)	189	296	416.63	5.041	34.76	1.31	0.657
16	McCubrey and Singh ⁴¹ (η)	182	295–478	416.45	5.041	34.70	1.32	0.637
17	Ellis and Raw ⁴² (η)	179	470–973	417.64	5.039	34.91	1.34	0.639
18	Dawe <i>et al.</i> ⁶³ (η)	172	293–873	417.18	5.040	34.92	1.32	0.663
19	Kestin <i>et al.</i> ⁹² (η)	188	296–302	416.53	5.041	34.71	1.32	0.659
20	Hellemans <i>et al.</i> ⁶⁵ (η)	183	298–573	417.10	5.040	34.91	1.32	0.665
21	Veda and Kigoshi ⁹³ (η)	182	273–346	418.41	5.036	35.30	1.29	0.640
22	Timrot <i>et al.</i> ⁹⁴ (η)	182	299–523	416.80	5.041	34.79	1.31	0.669
23	Kestin <i>et al.</i> ^{66,95,96a} (η)	175 ^a	296–477	417.13	5.041	35.09	1.27	0.650
24	Abe <i>et al.</i> ⁹⁷ (η)	188	423–468	417.12	5.040	34.94	1.30	0.647
25	Harris <i>et al.</i> ⁹⁸ (η)	183	218–302	417.58	5.038	35.04	1.30	0.661
26	Tanaka <i>et al.</i> ⁹⁹ (η)	187	298–348	416.72	5.041	34.77	1.32	0.660
27	Hoogland <i>et al.</i> ¹⁰⁰ (η)	185	298–333	416.45	5.041	34.69	1.32	0.663
28	Strehlow and Vogel ⁸⁰ (η)	181	298–673	408.43	5.057	32.06	1.42	0.605
29	Refs. 32–46 (B)	87	199–550	418.45	5.079	38.47	1.06	0.570
30	Refs. 14–31 (η)	103	218–973	323.56	5.288	27.27	0.10	0.676
31	Best solution (B + η)	190	199–973	416.79	5.041	34.79	1.31	0.657

^aFor the sake of clearer representation three works of Kestin and co-authors were shown in Fig. 4 by the same symbol.

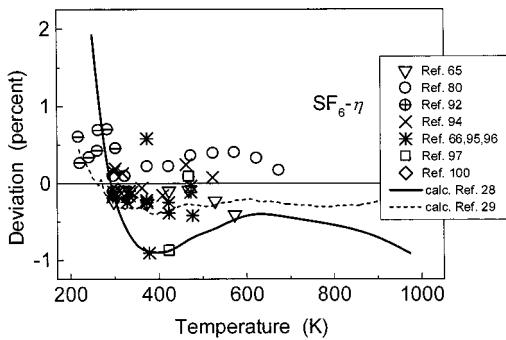


FIG. 4. Comparison of $\eta(T)$ calculated by means of ITDP (zero line) with the tabulated values of Boushehri *et al.*²⁸ and Trengove and Wakeham.²⁹ The deviations of the most accurate measurements used in the minimization are also plotted.

The calculations of $B(T)$ by Boushehri *et al.*²⁸ are compared with our results in Fig. 5. The deviations are within the frame of the accuracy of $\pm 6 \text{ cm}^3 \text{ mol}^{-1}$ given by Boushehri *et al.*²⁸ In the same figure the deviations of $B(T)$ derived from refractivities measured by Häusler and Kerl¹²⁵ (empty circles) are shown. The old data of Mears *et al.*¹²⁶ (full circles) are also presented in Fig. 5.

4.1.3. Comparison with the MMSV potential

A large variety of (12-6) LJ potentials has been suggested for SF₆-SF₆ interactions by different authors since 1951 (see for example the review by Aziz *et al.*⁶). A brief look shows that r_m varies from 4.705 to $6.720 \times 10^{-10} \text{ m}$, and ϵ from 155 to 494 K. The most successful pair potential for SF₆ has been introduced in 1991 by Aziz *et al.* It proved to be well suited for simultaneously fitting $B(T)$ and $\eta(T)$, which makes a comparison between it and ITDP straightforward.

In Fig. 6 we plotted two ITDP calculated at 300 and 600 K together with the MMSV potential.⁶ A large discrepancy in their shapes is observed at short distances. The MMSV has a much smaller equilibrium distance of $4.705 \times 10^{-10} \text{ m}$ compared to our $5.04 \times 10^{-10} \text{ m}$, while the potential well depth of the MMSV potential is larger compared to our solution (450 K versus 416.8 K). The MMSV is also much steeper. Its short distance behavior can be approximated with a repulsive

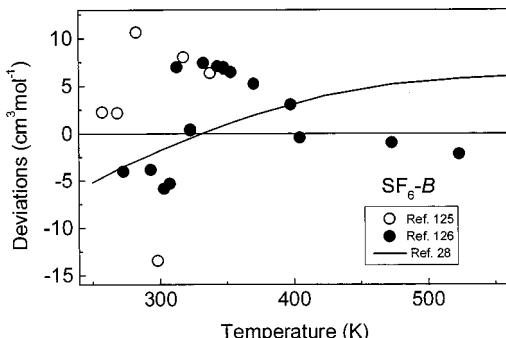


FIG. 5. Comparison of $B(T)$ calculated by means of ITDP (zero line) with the tabulated values of Boushehri *et al.*²⁸

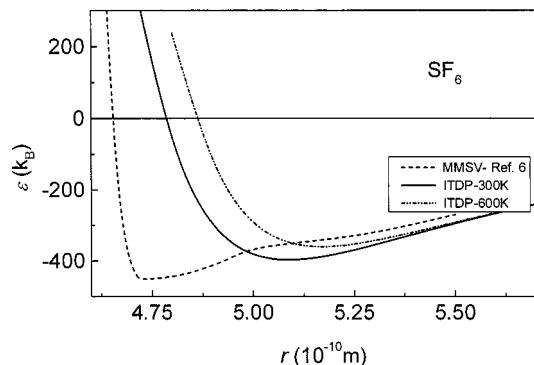


FIG. 6. Comparison of the ITDP (at $T=300 \text{ K}$ and $T=600 \text{ K}$) with the MMSV potential.

parameter of $n \approx 120$. This value is extremely large although it is known that for some other HGM $n > 12$ results (e.g., CF₄: $n = 39$)^{127,128}. This is considered to be one of the main reasons for the failure of the MMSV to reproduce the CILS spectra of SF₆.³ The crystallographic data of Lichtenhaller and Schäfer¹²⁹ ($r_m = 5.02 \times 10^{-10} \text{ m}$) seems to support our value ($5.04 \times 10^{-10} \text{ m}$).

4.1.4. Summary

The discussion is summarized in Table 17. We have confirmed the reliability and universality of the ITDP. We come to the conclusion that our ITDP approach in many aspects is superior to hitherto published potentials of heavy globular molecules.

5. Deviation Plots

The deviation plots are shown in Figs. 7–28. Absolute deviations for $B_{\text{exp}} - B_{\text{calc}}$ (in $\text{cm}^3 \text{ mol}^{-1}$) are presented in Figs. 7–17. In the case of the viscosity relative deviations $\eta_{\text{exp}} - \eta_{\text{calc}}$ (in percent) are plotted against the temperature in Figs. 18–28.

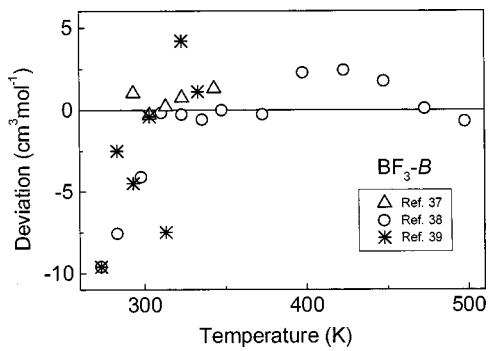
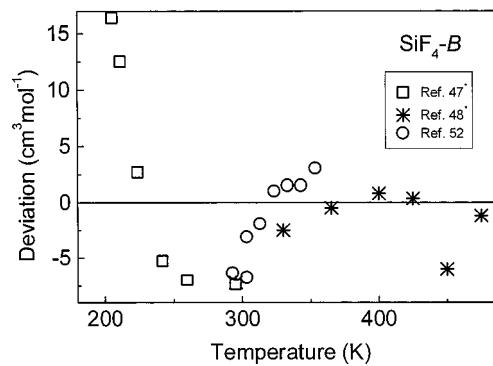
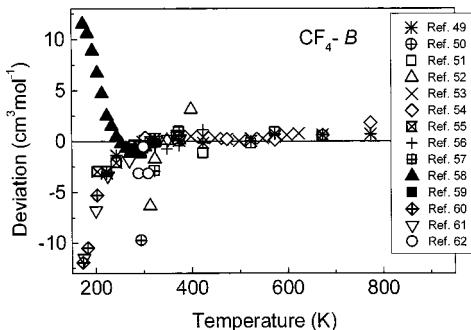
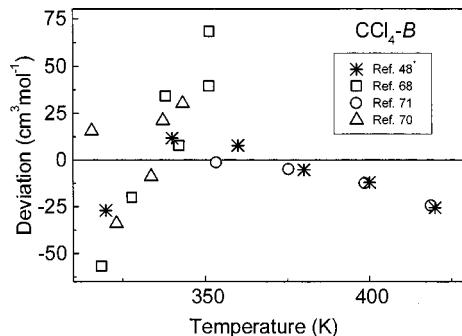
As a consequence of the large absolute values of $B(T)$ in some pVT -second virial coefficient plots deviations at low temperatures are looking rather large. As already stated, the minimization has been performed for the weighted relative deviations and the obtained RMS for the majority of gases is less or close to $\pm 1 a_{\text{exp}}$. RMS of about $\pm 2 a_{\text{exp}}$ (for MoF₆, WF₆, UF₆) appear when only a small number of scattered experimental data are available. All of these plots serve as a basis for a reasonable determination of the ITDP and reliable prediction of equilibrium and transport properties for all considered gases in a wide range of temperatures.

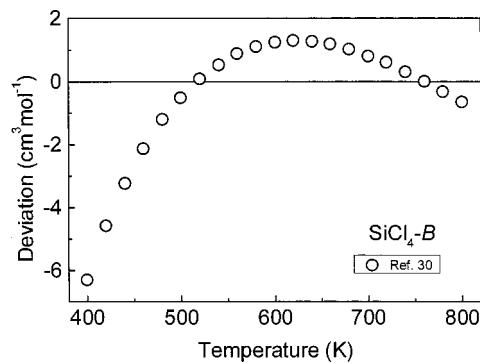
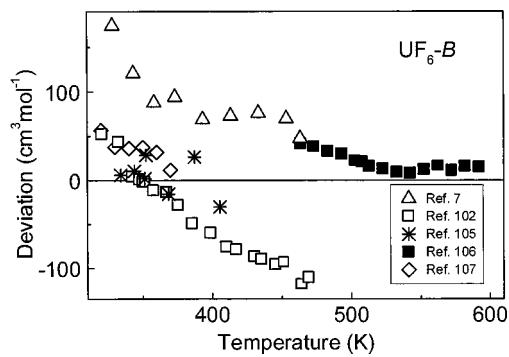
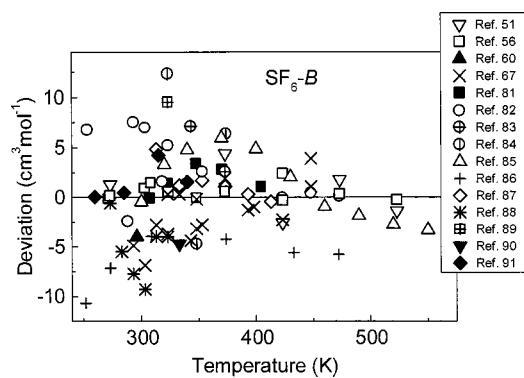
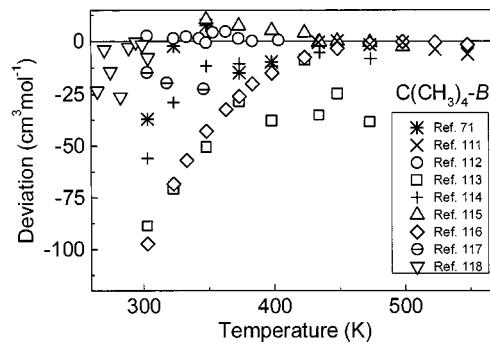
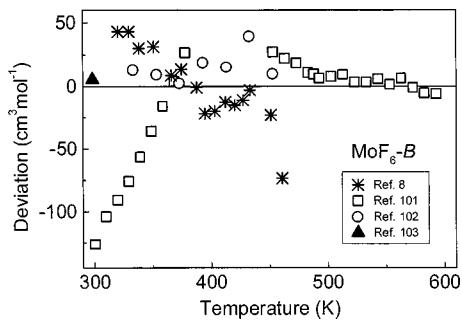
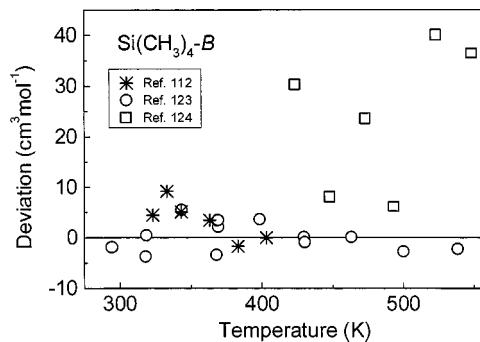
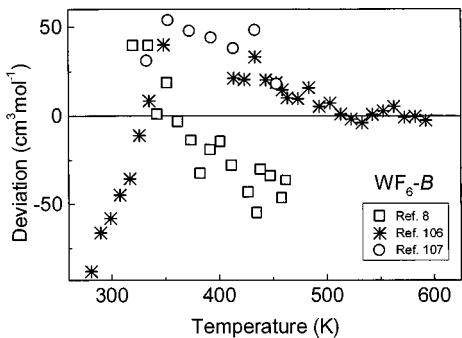
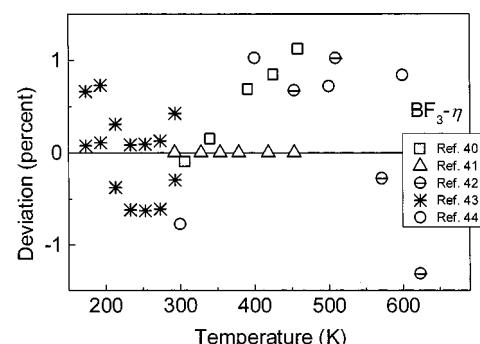
6. Tabulations

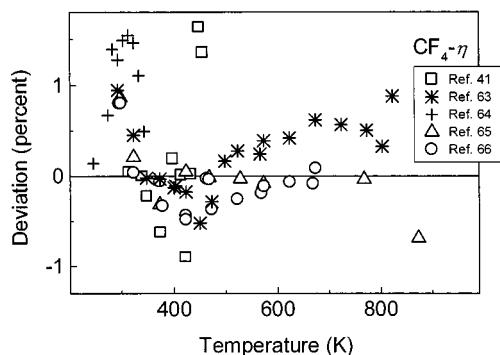
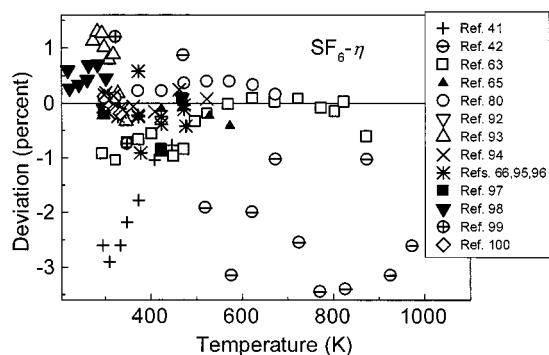
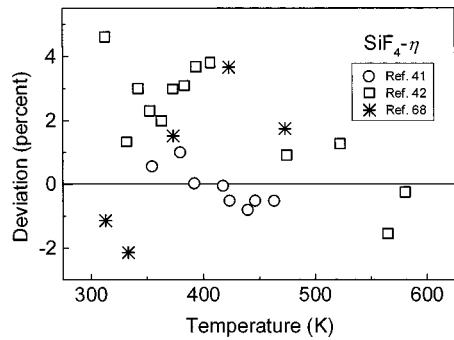
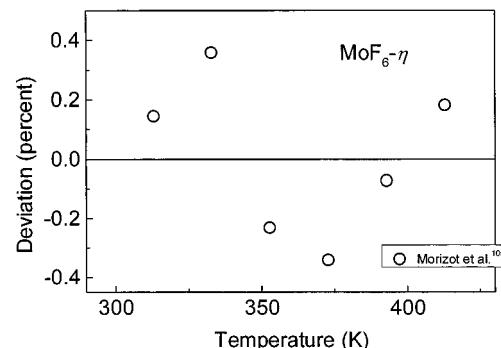
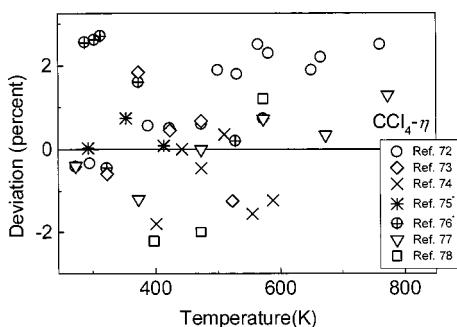
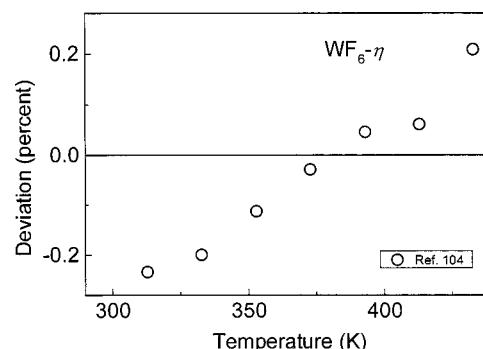
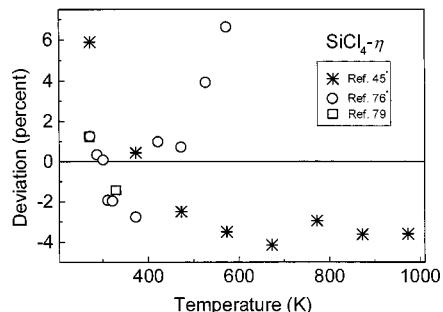
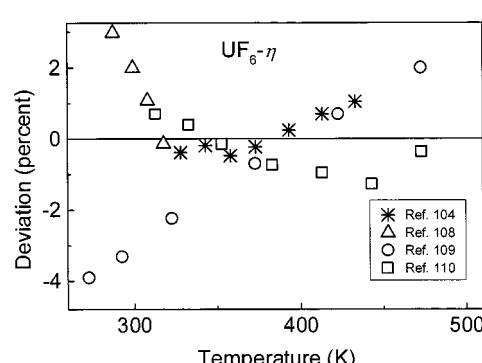
The ITDP approach and procedures described in the preceding sections have been employed to generate tables of recommended equilibrium distance, potential depth well,

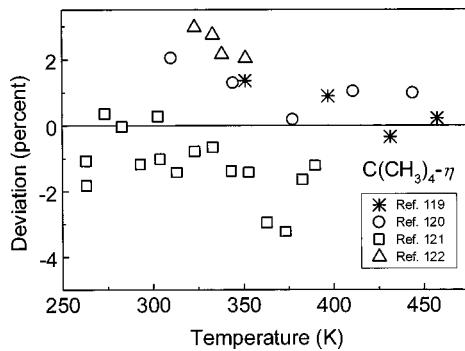
TABLE 17. Comparison between MMSV potential and ITDP

	MMSV	ITDP
Simultaneous fit of B and η	Very good	Very good
Potential shape	Morse–Morse + Spline + Van der Waals	($n - 6$) LJ potential
Input data	Sets of experimental data Many constants needed to fix different areas of the patch potential	Sets of experimental data Normal vibrational frequencies
C_6	Not known	Good agreement with r_m from crystallographic data ¹²⁹
Proofs from other fields	Not known	Pure gases: BF_3 , CF_4 , CCl_4 , SiF_4 , SiCl_4 , SF_6 , UF_6 , WF_6 , MoF_6 , $\text{C}(\text{CH}_3)_4$, $\text{Si}(\text{CH}_3)_4$. Mixtures: $\text{CH}_4\text{--CF}_4$, $\text{CH}_4\text{--SF}_6$, $\text{CF}_4\text{--SF}_6$, $\text{UF}_6\text{--WF}_6$, $\text{UF}_6\text{--MoF}_6$, $\text{WF}_6\text{--MoF}_6$, $\text{CH}_4\text{--C}(\text{CH}_3)_4$
Successfully applied to other HGM and their mixtures	Not known	

FIG. 7. Deviation plot for $B(T)$ of BF_3 .FIG. 9. Deviation plot for $B(T)$ of SiF_4 .FIG. 8. Deviation plot for $B(T)$ of CF_4 .FIG. 10. Deviation plot for $B(T)$ of CCl_4 .

FIG. 11. Deviation plot for $B(T)$ of SiCl_4 .FIG. 15. Deviation plot for $B(T)$ of UF_6 .FIG. 12. Deviation plot for $B(T)$ of SF_6 .FIG. 16. Deviation plot for $B(T)$ of $\text{C}(\text{CH}_3)_4$.FIG. 13. Deviation plot for $B(T)$ of MoF_6 .FIG. 17. Deviation plot for $B(T)$ of $\text{Si}(\text{CH}_3)_4$.FIG. 14. Deviation plot for $B(T)$ of WF_6 .FIG. 18. Deviation plot for $\eta(T)$ of BF_3 .

FIG. 19. Deviation plot for $\eta(T)$ of CF_4 .FIG. 23. Deviation plot for $\eta(T)$ of SF_6 .FIG. 20. Deviation plot for $\eta(T)$ of SiF_4 .FIG. 24. Deviation plot for $\eta(T)$ of MoF_6 .FIG. 21. Deviation plot for $\eta(T)$ of CCl_4 .FIG. 25. Deviation plot for $\eta(T)$ of WF_6 .FIG. 22. Deviation plot for $\eta(T)$ of SiCl_4 .FIG. 26. Deviation plot for $\eta(T)$ of UF_6 .

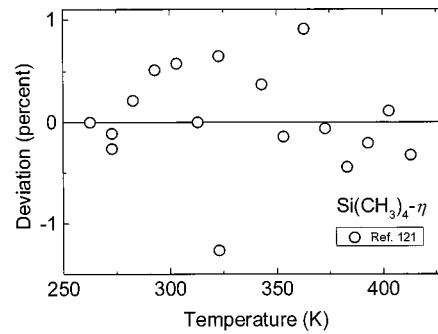
FIG. 27. Deviation plot for $\eta(T)$ of $\text{C}(\text{CH}_3)_4$.

(pVT)-second virial coefficient, viscosity, and self-diffusion in the temperature range between 200 and 900 K for BF_3 , SiF_4 , CCl_4 , SiCl_4 , MoF_6 , WF_6 , UF_6 , $\text{C}(\text{CH}_3)_4$, and $\text{Si}(\text{CH}_3)_4$, and 170–1000 K for CF_4 and SF_6 . The temperature ranges for the last two gases have been extended in accordance with the existence of measured data in these areas. The values of the ITDP parameters at $T=0$ K are given in Table 18. Their uncertainties are evaluated by means of the covariance-variance matrix.

All 11 property tables 19–40 (the odd numbered tables from 19 to 40) are identical in their structure. The step of 10 K between each two successive temperatures allows linear approximation. The PP could be also used to estimate other potential-dependent properties for pure substances or multi-component mixtures needed for interpretation of the experimental results in different fields, such as spectroscopy, speed-of-sound measurements, cluster formation, etc. For further calculations the quantities $r_m/(10^{-10} \text{ m})$, $\varepsilon/(k_B \text{ K})$, $\eta/(\mu\text{Pa s})$, and $\rho D/(\text{g m}^{-1} \text{ s}^{-1})$ are fitted to a polynomial in powers of the temperature T of the form

$$P = \sum_{i=1}^4 A_i (T/K)^{i-1}, \quad (6)$$

whereas the second pVT -virial coefficient is represented by

FIG. 28. Deviation plot for $\eta(T)$ of $\text{Si}(\text{CH}_3)_4$.

$$B(T)/(\text{cm}^3 \text{ mol}^{-1}) = \sum_{i=1}^4 A_i (T/\text{K})^{1-i}. \quad (7)$$

The fit parameters A_i are given in the even numbered tables from 20–40. It should be mentioned that the fits are only valid in the temperature ranges for which the corresponding properties are calculated (see Tables 19–40).

7. Conclusion

Here we present self-consistent equilibrium and transport property data for 11 heavy globular gases calculated by means of an ITDP. With the exception of carbon tetrachloride, we have observed the same trend in the temperature dependence of the potential parameters: the equilibrium distance increases and the potential well depth decreases when the temperature is increasing. The application of the ITDP approach to any HGM in this moment is restricted only by the lack of experimental data.

CCl_4 has demonstrated a paradoxical behavior: decreasing $r_m(T)$ and increasing $\varepsilon(T)$. This fact has been carefully explored and confirmed for the existing set of experimental data. It deserves further experimental and theoretical investigation since a similar temperature influence has been reported earlier by Hoogeveen *et al.*²⁰ for polar molecules.

TABLE 18. ITDP parameters at $T=0$ K

	Gas	$m/\text{a.u.}$	ε/k_B	$r_m/10^{-10} \text{ m}$	n	$\delta/10^{-12} \text{ m}$	$\text{RMS}/a_{\text{exp}}$
BF_3	boron trifluoride	67.81	310.5(2.1)	4.196(6)	23.00(31)	9.57 ± 0.35	0.686
CF_4	carbon tetrafluoride	88.00	328.4(1.1)	4.329(2)	52.71(63)	1.29(3)	0.701
SiF_4	silicon tetrafluoride	104.08	200.2(1.1)	5.270(10)	12.83(11)	2.09(17)	0.691
CCl_4	carbon tetrachloride	153.82	696.4(3.8)	5.589(6)	18.6(2.2)	-0.55(14)	0.640
SiCl_4	silicon tetrachloride	169.90	775.2(1.1)	5.715(10)	26.05(11)	1.98(17)	0.596
SF_6	sulfur hexafluoride	146.06	417.80(87)	5.041(3)	34.76(33)	1.31(3)	0.657
MoF_6	molybdenum hexafluoride	209.93	827.3(1.4)	4.995(8)	28.19(24)	1.94(3)	1.568
WF_6	tungsten hexafluoride	297.83	712.8(1.1)	5.076(7)	17.22(13)	3.36(3)	1.966
UF_6	uranium hexafluoride	352.02	1040.0(2.3)	4.992(5)	27.87(30)	2.26(3)	2.061
$\text{C}(\text{CH}_3)_4$	tetramethyl methane, TMM	72.14	586.32(42)	5.779(3)	28.02(12)	1.41(3)	1.201
$\text{Si}(\text{CH}_3)_4$	tetramethyl silane, TMS	88.22	674.74(91)	5.905(4)	20.79(11)	1.88(3)	0.769

TABLE 19. Potential parameters $r_m(T)$ and $\varepsilon(T)$ and recommended thermophysical properties of BF_3

T/K	$r_m/10^{-8} \text{ cm}$	$\varepsilon/k_B/\text{K}$	$-B(T)/\text{cm}^3 \text{ mol}^{-1}$	$\eta/\mu\text{Pa s}$	$\rho D/\text{g m}^{-1} \text{ s}^{-1}$
200	4.209 859	304.3778	243.427 63	11.6420	15.2813
210	4.212 566	303.2062	220.320 61	12.1782	15.9784
220	4.215 527	301.9309	200.226 40	12.7150	16.6736
230	4.218 703	300.5696	182.565 23	13.2519	17.3672
240	4.222 086	299.1271	166.891 85	13.7875	18.0588
250	4.225 678	297.6051	152.873 10	14.3206	18.7471
260	4.229 468	296.0083	140.261 59	14.8518	19.4289
270	4.233 445	294.3438	128.858 47	15.3827	20.0998
280	4.237 597	292.6177	118.500 86	15.9134	20.7595
290	4.241 914	290.8353	109.050 11	16.4417	21.4130
300	4.246 389	289.0015	100.388 80	16.9652	22.0661
310	4.251 011	287.1213	92.418 80	17.4833	22.7186
320	4.255 771	285.1995	85.057 75	17.9960	23.3682
330	4.260 663	283.2405	78.236 66	18.5035	24.0117
340	4.265 677	281.2487	71.896 87	19.0060	24.6455
350	4.270 807	279.2279	65.988 02	19.5038	25.2669
360	4.276 045	277.1818	60.466 43	19.9968	25.8766
370	4.281 385	275.1141	55.293 85	20.4849	26.4761
380	4.286 820	273.0278	50.436 96	20.9681	27.0676
390	4.292 345	270.9262	45.866 57	21.4463	27.6533
400	4.297 953	268.8120	41.556 99	21.9189	28.2337
410	4.303 639	266.6879	37.485 53	22.3852	28.8083
420	4.309 399	264.5563	33.632 10	22.8441	29.3766
430	4.315 228	262.4196	29.978 82	23.2949	29.9380
440	4.321 120	260.2797	26.509 67	23.7376	30.4921
450	4.327 073	258.1388	23.210 29	24.1727	31.0382
460	4.333 081	255.9985	20.067 81	24.6013	31.5760
470	4.339 142	253.8606	17.070 62	25.0241	32.1048
480	4.345 251	251.7266	14.208 21	25.4412	32.6245
490	4.351 406	249.5978	11.471 07	25.8523	33.1350
500	4.357 603	247.4756	8.850 60	26.2571	33.6362
510	4.363 840	245.3612	6.338 93	26.6554	34.1283
520	4.370 112	243.2556	3.928 90	27.0471	34.6116
530	4.376 419	241.1599	1.613 94	27.4321	35.0865
540	4.382 758	239.0748	-0.611 92	27.8105	35.5534
550	4.389 125	237.0013	-2.754 19	28.1822	36.0130
560	4.395 520	234.9401	-4.817 95	28.5474	36.4661
570	4.401 939	232.8918	-6.807 83	28.9060	36.9133
580	4.408 381	230.8573	-8.728 14	29.2582	37.3549
590	4.414 844	228.8370	-10.582 84	29.6042	37.7907
600	4.421 328	226.8308	-12.375 62	29.9439	38.2205
610	4.427 832	224.8390	-14.109 86	30.2778	38.6440
620	4.434 349	222.8636	-15.788 73	30.6060	39.0610
630	4.440 878	220.9049	-17.415 15	30.9288	39.4711
640	4.447 423	218.9615	-18.991 86	31.2463	39.8744
650	4.453 980	217.0345	-20.521 39	31.5585	40.2711
660	4.460 548	215.1242	-22.006 11	31.8654	40.6612
670	4.467 125	213.2307	-23.448 23	32.1669	41.0451
680	4.473 710	211.3544	-24.849 81	32.4632	41.4229
690	4.480 303	209.4953	-26.212 79	32.7542	41.7950
700	4.486 901	207.6537	-27.538 96	33.0402	42.1612
710	4.493 504	205.8295	-28.830 03	33.3214	42.5217
720	4.500 111	204.0231	-30.087 57	33.5980	42.8763
730	4.506 720	202.2344	-31.313 08	33.8703	43.2250
740	4.513 331	200.4635	-32.507 96	34.1385	43.5679
750	4.519 943	198.7105	-33.673 51	34.4026	43.9050
760	4.526 554	196.9755	-34.810 99	34.6626	44.2367
770	4.533 164	195.2585	-35.921 54	34.9185	44.5630
780	4.539 771	193.5596	-37.006 25	35.1701	44.8842
790	4.546 375	191.8788	-38.066 14	35.4176	45.2005
800	4.55 297	190.2162	-39.102 18	35.6610	45.5120
810	4.559 568	188.5718	-40.115 32	35.9004	45.8189
820	4.566 155	186.9453	-41.106 44	36.1361	46.1211
830	4.572 736	185.3368	-42.076 40	36.3682	46.4190
840	4.579 309	183.7464	-43.025 93	36.5968	46.7112

TABLE 19. Potential parameters $r_m(T)$ and $\varepsilon(T)$ and recommended thermophysical properties of BF_3 —Continued

T/K	$r_m/10^{-8} \text{ cm}$	$\varepsilon/k_B/\text{K}$	$-B(T)/\text{cm}^3 \text{ mol}^{-1}$	$\eta/\mu\text{Pa s}$	$\rho D/\text{g m}^{-1} \text{ s}^{-1}$
850	4.585 872	182.1743	-43.955 67	36.8221	46.9987
860	4.592 422	180.6208	-44.866 18	37.0441	47.2821
870	4.598 957	179.0864	-45.758 04	37.2630	47.5614
880	4.605 478	177.5702	-46.632 05	37.4786	47.8366
890	4.611 990	176.0712	-47.489 19	37.6910	48.1078
900	4.618 497	174.5880	-48.330 40	37.9003	48.3749

TABLE 20. Fit parameters according to Eqs. (6) and (7) for BF_3

Property	A_1	A_2	A_3	A_4
$r_m/10^{-10} \text{ m}$	4.1710(18)	$1.1(1.1) \times 10^{-5}$	$9.50(22) \times 10^{-7}$	$-4.57(13) \times 10^{-10}$
$\varepsilon/k_B/\text{K}$	329.6(1.1)	-0.0713(68)	-0.000 275(13)	$1.824(79) \times 10^{-7}$
$-B(T)/\text{cm}^3 \text{ mol}^{-1}$	121.23(35)	$-6.919(44) \times 10^4$	$3.96(17) \times 10^6$	$-9.44(19) \times 10^8$
$\eta/\mu\text{Pa s}$	-1.59(11)	0.072 47(67)	$-3.60(13) \times 10^{-5}$	$4.65(80) \times 10^{-9}$
$\rho D/\text{g m}^{-1} \text{ s}^{-1}$	-1.433(72)	0.092 65(46)	$-4.982(89) \times 10^{-5}$	$9.24(54) \times 10^{-9}$

TABLE 21. Potential parameters $r_m(T)$ and $\varepsilon(T)$ and recommended thermophysical properties of CF_4

T/K	$r_m/10^{-8} \text{ cm}$	$\varepsilon/k_B/\text{K}$	$-B(T)/\text{cm}^3 \text{ mol}^{-1}$	$\eta/\mu\text{Pa s}$	$\rho D/\text{g m}^{-1} \text{ s}^{-1}$
170	4.330 706	327.6646	311.686 85	10.8668	14.0600
180	4.331 187	327.4464	275.875 47	11.3999	14.7532
190	4.331 684	327.2209	245.838 99	11.9304	15.4406
200	4.332 199	326.9842	221.193 22	12.4581	16.1224
210	4.332 779	326.7248	199.346 76	12.9835	16.7989
220	4.333 422	326.4343	180.350 16	13.5058	17.4683
230	4.334 122	326.1181	163.677 85	14.0243	18.1286
240	4.334 872	325.7797	148.924 01	14.5387	18.7782
250	4.335 654	325.4274	135.773 62	15.0496	19.4185
260	4.336 486	325.0527	123.979 96	15.5580	20.0509
270	4.337 360	324.6597	113.344 63	16.0646	20.6777
280	4.338 270	324.2517	103.706 01	16.5685	21.3007
290	4.339 211	323.8300	94.930 31	17.0681	21.9223
300	4.340 183	323.3950	86.906 08	17.5619	22.5443
310	4.341 186	322.9471	79.540 18	18.0501	23.1635
320	4.342 218	322.4868	72.754 25	18.5337	23.7739
330	4.343 277	322.0150	66.482 03	19.0136	24.3699
340	4.344 363	321.5327	60.667 03	19.4902	24.9508
350	4.345 471	321.0408	55.260 77	19.9630	25.5189
360	4.346 602	320.5402	50.221 35	20.4320	26.0773
370	4.347 752	320.0316	45.512 34	20.8967	26.6290
380	4.348 922	319.5155	41.101 99	21.3569	27.1777
390	4.350 109	318.9927	36.962 47	21.8122	27.7272
400	4.351 313	318.4635	33.069 35	22.2625	28.2778
410	4.352 532	317.9287	29.400 99	22.7078	28.8277
420	4.353 765	317.3888	25.938 29	23.1484	29.3747
430	4.355 011	316.8442	22.664 20	23.5842	29.9163
440	4.356 270	316.2954	19.563 53	24.0154	30.4498
450	4.357 539	315.7429	16.622 66	24.4421	30.9725
460	4.358 819	315.1870	13.829 37	24.8645	31.4842
470	4.360 109	314.6281	11.172 66	25.2827	31.9861
480	4.361 407	314.0667	8.642 59	25.6968	32.4794
490	4.362 713	313.5029	6.230 16	26.1070	32.9658
500	4.364 027	312.9371	3.927 23	26.5133	33.4467

TABLE 21. Potential parameters $r_m(T)$ and $\varepsilon(T)$ and recommended thermophysical properties of CF_4 —Continued

T/K	$r_m/10^{-8}$ cm	$\varepsilon/k_B/\text{K}$	$-B(T)/\text{cm}^3 \text{ mol}^{-1}$	$\eta/\mu\text{Pa s}$	$\rho D/\text{g m}^{-1} \text{ s}^{-1}$
510	4.365 347	312.3696	1.726 35	26.9160	33.9237
520	4.36 667	311.8008	-0.379 22	27.3150	34.3973
530	4.368 006	311.2307	-2.395 68	27.7101	34.8674
540	4.369 343	310.6598	-4.328 67	28.1012	35.3341
550	4.370 684	310.0881	-6.183 38	28.4881	35.7976
560	4.372 029	309.5160	-7.964 57	28.8707	36.2577
570	4.373 378	308.9436	-9.676 63	29.2490	36.7146
580	4.374 730	308.3712	-11.323 59	29.6229	37.1682
590	4.376 085	307.7989	-12.909 19	29.9929	37.6182
600	4.377 442	307.2268	-14.436 86	30.3589	38.0646
610	4.378 801	306.6553	-15.909 80	30.7214	38.5072
620	4.380 161	306.0843	-17.330 97	31.0805	38.9458
630	4.381 522	305.5142	-18.703 12	31.4363	39.3803
640	4.382 884	304.9451	-20.028 80	31.7888	39.8108
650	4.384 246	304.3770	-21.310 37	32.1380	40.2371
660	4.385 608	303.8102	-22.550 07	32.4841	40.6593
670	4.386 970	303.2449	-23.749 95	32.8269	41.0774
680	4.388 331	302.6811	-24.911 94	33.1665	41.4912
690	4.389 691	302.1190	-26.037 84	33.5030	41.9007
700	4.391 049	301.5588	-27.129 33	33.8364	42.3059
710	4.392 405	301.0006	-28.188 00	34.1667	42.7067
720	4.393 759	300.4445	-28.188 00	34.4939	43.1031
730	4.395 110	299.8908	-29.215 33	34.8181	43.4950
740	4.396 458	299.3396	-30.212 70	35.1393	43.8825
750	4.397 802	298.7910	-31.181 41	35.4576	44.2660
760	4.399 143	298.2451	-32.122 70	35.7730	44.6455
770	4.400 479	297.7021	-33.037 71	36.0855	45.0213
780	4.401 810	297.1623	-33.927 53	36.3952	45.3937
790	4.403 136	296.6257	-34.793 17	36.7022	45.7629
800	4.404 457	296.0926	-35.635 60	37.0066	46.1291
810	4.405 771	295.5630	-36.455 71	37.3082	46.4926
820	4.407 079	295.0369	-37.254 38	37.6074	46.8537
830	4.408 381	294.5145	-38.032 46	37.9040	47.2126
840	4.409 676	293.9959	-38.790 72	38.1982	47.5696
850	4.410 963	293.4816	-39.529 89	38.4900	47.9246
860	4.412 241	292.9722	-40.250 56	38.7795	48.2776
870	4.413 508	292.4680	-40.953 31	39.0667	48.6287
880	4.414 765	291.9685	-41.638 68	39.3518	48.9778
890	4.416 016	291.4727	-42.960 38	39.6347	49.3248
900	4.417 263	290.9791	-43.598 44	39.9156	49.6698
910	4.418 496	290.4924	-44.084 46	40.2088	50.0312
920	4.419 719	290.0104	-44.693 89	40.4859	50.3722
930	4.420 932	289.5335	-45.289 75	40.7611	50.7111
940	4.422 132	289.0621	-45.872 45	41.0344	51.0478
950	4.423 320	288.5967	-46.442 41	41.3059	51.3823
960	4.424 494	288.1377	-46.999 99	41.5755	51.7145
970	4.425 653	287.6851	-47.545 56	41.8432	52.0446
980	4.426 802	287.2375	-48.079 48	42.1091	52.3725
990	4.427 943	286.7936	-48.714 79	42.3731	52.6981
1000	4.429 080	286.3520	-49.113 66	42.6351	53.0215

TABLE 22. Fit parameters according to Eqs. (6) and (7) for CF_4

Property	A_1	A_2	A_3	A_4
$r_m/10^{-10}$ m	4.323 99(35)	$3.1(2.2) \times 10^{-6}$	$2.044(41) \times 10^{-7}$	$-1.028(23) \times 10^{-10}$
$\varepsilon/k_B/\text{K}$	331.18(18)	-0.0052(11)	$-8.47(21) \times 10^{-5}$	$4.54(12) \times 10^{-8}$
$-B(T)/\text{cm}^3 \text{ mol}^{-1}$	97.43(37)	$-4.767(45) \times 10^4$	$-4.2(1.6) \times 10^5$	$-5.59(17) \times 10^8$
$\eta/\mu\text{Pa s}$	0.561(27)	0.065 10(17)	$-2.984(31) \times 10^{-5}$	$6.80(18) \times 10^{-9}$
$\rho D/\text{g m}^{-1} \text{ s}^{-1}$	0.967(25)	0.084 31(15)	$-4.514(28) \times 10^{-5}$	$1.290(16) \times 10^{-8}$

TABLE 23. Potential parameters $r_m(T)$ and $\varepsilon(T)$ and recommended thermophysical properties of SiF₄

T/K	$r_m/10^{-8}$ cm	ε/k_B /K	$-B(T)/\text{cm}^3 \text{ mol}^{-1}$	$\eta/\mu\text{Pa s}$	$\rho D/\text{g m}^{-1} \text{ s}^{-1}$
200	5.291 854	195.2902	304.888 38	11.0886	14.7315
210	5.294 568	194.6904	278.206 32	11.6237	15.4394
220	5.297 304	194.0878	254.602 32	12.1212	16.1228
230	5.300 084	193.4777	233.567 48	12.6125	16.7975
240	5.302 929	192.8560	214.697 61	13.1312	17.4812
250	5.305 843	192.2212	197.672 20	13.6770	18.1721
260	5.308 815	191.5765	182.236 01	14.2290	18.8561
270	5.311 831	190.9248	168.179 50	14.7603	19.5156
280	5.314 878	190.2690	155.328 63	15.2531	20.1404
290	5.317 950	189.6104	143.535 92	15.7170	20.7425
300	5.321 046	188.9495	132.676 07	16.1677	21.3391
310	5.324 164	188.2865	122.642 78	16.6219	21.9481
320	5.327 303	187.6219	113.345 35	17.0820	22.5687
330	5.330 459	186.9563	104.706 11	17.5430	23.1891
340	5.333 630	186.2903	96.658 04	17.9987	23.7962
350	5.336 813	185.6247	89.142 95	18.4463	24.3837
360	5.340 006	184.9599	82.110 01	18.8879	24.9563
370	5.343 206	184.2962	75.514 50	19.3266	25.5203
380	5.346 412	183.6341	69.317 07	19.7644	26.0810
390	5.349 623	182.9738	63.482 97	20.2003	26.6383
400	5.352 837	182.3155	57.981 38	20.6327	27.1914
410	5.356 054	181.6596	52.784 84	21.0597	27.7389
420	5.359 271	181.0062	47.868 88	21.4791	28.2795
430	5.362 488	180.3556	43.211 55	21.8885	28.8120
440	5.365 704	179.7080	38.793 13	22.2856	29.3348
450	5.368 918	179.0634	34.595 83	22.6710	29.8483
460	5.372 130	178.4222	30.603 62	23.0464	30.3537
470	5.375 337	177.7843	26.801 97	23.4143	30.8524
480	5.378 540	177.1500	23.177 66	23.7770	31.3460
490	5.381 738	176.5193	19.718 71	24.1373	31.8361
500	5.384 931	175.8924	16.414 17	24.4980	32.3247
510	5.388 117	175.2692	13.254 04	24.8601	32.8121
520	5.391 296	174.6500	10.229 18	25.2228	33.2983
530	5.394 468	174.0348	7.331 17	25.5854	33.7828
540	5.397 632	173.4236	4.552 32	25.9471	34.2653
550	5.400 788	172.8165	1.885 53	26.3068	34.7454
560	5.403 935	172.2135	-0.675 75	26.6637	35.2227
570	5.407 072	171.6148	-3.137 55	27.0172	35.6964
580	5.410 200	171.0204	-5.505 45	27.3668	36.1656
590	5.413 317	170.4303	-7.784 63	27.7121	36.6293
600	5.416 424	169.8446	-9.979 87	28.0527	37.0863
610	5.419 520	169.2633	-12.095 63	28.3882	37.5357
620	5.422 604	168.6865	-14.136 03	28.7182	37.9765
630	5.425 676	168.1143	-16.104 92	29.0434	38.4100
640	5.428 735	167.5466	-18.005 87	29.3648	38.8377
650	5.431 782	166.9837	-19.842 24	29.6832	39.2613
660	5.434 814	166.4254	-21.617 14	29.9998	39.6826
670	5.437 832	165.8719	-23.333 47	30.3155	40.1035
680	5.440 836	165.3233	-24.993 95	30.6306	40.5244
690	5.443 823	164.7797	-26.601 15	30.9445	40.9446
700	5.446 795	164.2410	-28.157 44	31.2566	41.3631
710	5.449 750	163.7074	-29.665 06	31.5661	41.7787
720	5.452 687	163.1790	-31.126 11	31.8723	42.1905
730	5.455 606	162.6559	-32.542 57	32.1745	42.5971
740	5.458 506	162.1380	-33.916 29	32.4719	42.9919
750	5.461 387	161.6256	-35.249 03	32.7645	43.3794
760	5.464 247	161.1187	-36.542 44	33.0529	43.7612
770	5.467 086	160.6173	-37.798 07	33.3375	44.1380
780	5.469 903	160.1217	-39.017 35	33.6187	44.5103
790	5.472 697	159.6318	-40.201 64	33.8972	44.8789
800	5.475 467	159.1479	-41.352 27	34.1733	45.2445
810	5.478 212	158.6699	-42.470 51	34.4475	45.6076
820	5.480 934	158.1977	-43.557 63	34.7198	45.9681
830	5.483 632	157.7313	-44.614 80	34.9902	46.3262
840	5.486 304	157.2709	-45.643 03	35.2589	46.6818

TABLE 23. Potential parameters $r_m(T)$ and $\varepsilon(T)$ and recommended thermophysical properties of SiF_4 —Continued

T/K	$r_m/10^{-8} \text{ cm}$	$\varepsilon/k_B/\text{K}$	$-B(T)/\text{cm}^3 \text{ mol}^{-1}$	$\eta/\mu\text{Pa s}$	$\rho D/\text{g m}^{-1} \text{ s}^{-1}$
850	5.488 948	156.8169	-46.643 08	35.5258	47.0352
860	5.491 560	156.3699	-47.615 64	35.7909	47.3863
870	5.494 137	155.9303	-48.561 43	36.0545	47.7352
880	5.496 684	155.4975	-49.481 77	36.3164	48.0819
890	5.499 209	155.0695	-50.378 43	36.5766	48.4265
900	5.501 723	154.6448	-51.253 14	36.8351	48.7687

TABLE 24. Fit parameters according to Eqs. (6) and (7) for SiF_4

Property	A_1	A_2	A_3	A_4
$r_m/10^{-10} \text{ m}$	5.237 74(43)	0.000 236 0(27)	$1.819(53) \times 10^{-7}$	$-1.316(32) \times 10^{-10}$
$\varepsilon/k_B/\text{K}$	208.29(11)	-0.061 57(72)	$-1.69(14) \times 10^{-5}$	$2.132(84) \times 10^{-8}$
$-B(T)/\text{cm}^3 \text{ mol}^{-1}$	126.30(16)	$-6.262(20) \times 10^4$	$-4.135(77) \times 10^6$	$-1.162(89) \times 10^8$
$\eta/\mu\text{Pa s}$	-1.091(80)	0.068 77(51)	$-4.178(99) \times 10^{-5}$	$1.361(60) \times 10^{-8}$
$\rho D/\text{g m}^{-1} \text{ s}^{-1}$	-0.591(95)	0.085 70(60)	$-4.60(12) \times 10^{-5}$	$1.310(70) \times 10^{-8}$

TABLE 25. Potential parameters $r_m(T)$ and $\varepsilon(T)$ and recommended thermophysical properties of CCl_4

T/K	$r_m/10^{-8} \text{ cm}$	$\varepsilon/k_B/\text{K}$	$-B(T)/\text{cm}^3 \text{ mol}^{-1}$	$\eta/\mu\text{Pa s}$	$\rho D/\text{g m}^{-1} \text{ s}^{-1}$
200	5.579 615	703.4477	4049.549 16	7.1492	9.1916
210	5.578 595	704.2198	3534.631 06	7.4453	9.5945
220	5.577 570	704.9969	3121.455 31	7.7413	9.9970
230	5.576 534	705.7825	2784.321 30	8.0370	10.3992
240	5.575 485	706.5802	2505.171 49	8.3317	10.8008
250	5.574 419	707.3910	2271.013 11	8.6246	11.2015
260	5.573 341	708.2122	2072.304 49	8.9153	11.6014
270	5.572 254	709.0413	1901.926 87	9.2049	12.0009
280	5.571 162	709.8756	1754.483 21	9.4945	12.4006
290	5.570 067	710.7139	1625.825 85	9.7851	12.8014
300	5.568 968	711.5557	1512.721 88	10.0775	13.2034
310	5.567 866	712.4009	1412.617 80	10.3716	13.6065
320	5.566 762	713.2488	1323.473 93	10.6673	14.0107
330	5.565 657	714.0991	1243.643 89	10.9645	14.4158
340	5.564 551	714.9510	1171.786 56	11.2631	14.8216
350	5.563 446	715.8039	1106.799 96	11.5628	15.2278
360	5.562 341	716.6573	1047.771 61	11.8636	15.6342
370	5.561 238	717.5109	993.940 36	12.1651	16.0406
380	5.560 136	718.3642	944.666 59	12.4673	16.4468
390	5.559 037	719.2171	899.409 28	12.7701	16.8527
400	5.557 940	720.0692	857.708 14	13.0734	17.2582
410	5.556 846	720.9202	819.169 29	13.3770	17.6630
420	5.555 755	721.7699	783.453 88	13.6809	18.0672
430	5.554 667	722.6181	750.268 95	13.9848	18.4704
440	5.553 584	723.4645	719.360 09	14.2886	18.8725
450	5.552 504	724.3089	690.505 38	14.5923	19.2735
460	5.551 429	725.1513	663.510 37	14.8958	19.6735
470	5.550 357	725.9913	638.204 04	15.1992	20.0727
480	5.549 291	726.8290	614.435 47	15.5026	20.4712
490	5.548 229	727.6641	592.070 93	15.8060	20.8692
500	5.547 172	728.4966	570.991 58	16.1095	21.2668

TABLE 25. Potential parameters $r_m(T)$ and $\varepsilon(T)$ and recommended thermophysical properties of CCl_4 —Continued

T/K	$r_m/10^{-8}$ cm	$\varepsilon/k_B/\text{K}$	$-B(T)/\text{cm}^3 \text{ mol}^{-1}$	$\eta/\mu\text{Pa s}$	$\rho D/\text{g m}^{-1} \text{ s}^{-1}$
510	5.546 119	729.3263	551.091 44	16.4130	21.6643
520	5.545 072	730.1531	532.275 76	16.7167	22.0618
530	5.544 030	730.9769	514.459 52	17.0205	22.4592
540	5.542 993	731.7977	497.566 30	17.3240	22.8564
550	5.541 962	732.6153	481.527 17	17.6272	23.2532
560	5.540 936	733.4297	466.279 82	17.9297	23.6494
570	5.539 915	734.2408	451.767 79	18.2315	24.0449
580	5.538 900	735.0484	437.939 82	18.5323	24.4394
590	5.537 891	735.8524	424.749 23	18.8318	24.8328
600	5.536 888	736.6528	412.153 47	19.1298	25.2248
610	5.535 890	737.4495	400.113 64	19.4268	25.6154
620	5.534 899	738.2423	388.594 12	19.7229	26.0046
630	5.533 914	739.0312	377.562 23	20.0187	26.3923
640	5.532 935	739.8159	366.987 94	20.3144	26.7785
650	5.531 963	740.5964	356.843 62	20.6105	27.1631
660	5.530 997	741.3724	347.103 77	20.9073	27.5462
670	5.530 039	742.1439	337.744 85	21.2055	27.9277
680	5.529 087	742.9107	328.745 09	21.5051	28.3076
690	5.528 143	743.6726	320.084 32	21.8058	28.6860
700	5.527 205	744.4294	311.743 84	22.1072	29.0632
710	5.526 276	745.1810	303.706 24	22.4088	29.4392
720	5.525 354	745.9270	295.955 39	22.7103	29.8142
730	5.524 441	746.6674	288.476 23	23.0110	30.1883
740	5.523 536	747.4020	281.254 74	23.3104	30.5618
750	5.522 639	748.1305	274.277 84	23.6081	30.9346
760	5.521 751	748.8527	267.533 29	23.9035	31.3071
770	5.520 871	749.5686	261.009 64	24.1968	31.6791
780	5.520 002	750.2776	254.696 14	24.4881	32.0505
790	5.519 141	750.9797	248.582 72	24.7774	32.4214
800	5.518 290	751.6746	242.659 95	25.0649	32.7916
810	5.517 449	752.3622	236.919 08	25.3507	33.1610
820	5.516 618	753.0427	231.351 91	25.6349	33.5297
830	5.515 796	753.7161	225.950 71	25.9177	33.8975
840	5.514 985	754.3820	220.708 05	26.1992	34.2644
850	5.514 184	755.0395	215.616 62	26.4796	34.6303
860	5.513 396	755.6876	210.669 53	26.7591	34.9952
870	5.512 620	756.3254	205.860 31	27.0378	35.3589
880	5.511 857	756.9544	201.183 81	27.3158	35.7214
890	5.511 101	757.5774	196.635 88	27.5935	36.0826
900	5.510 349	758.1976	192.212 61	27.8709	36.4425

TABLE 26. Fit parameters according to Eqs. (6) and (7) for CCl_4

Property	A_1	A_2	A_3	A_4
$r_m/10^{-10}$ m	5.600 82(12)	-0.000 100 15(74)	$-3.12(14) \times 10^{-8}$	$3.431(86) \times 10^{-11}$
$\varepsilon/k_B/\text{K}$	687.817(82)	0.071 97(52)	$3.33(10) \times 10^{-5}$	$-2.938(61) \times 10^{-8}$
$-B(T)/\text{cm}^3 \text{ mol}^{-1}$	331(13)	$-5.64(17) \times 10^5$	$1.338(64) \times 10^8$	$-3.905(75) \times 10^{10}$
$\eta/\mu\text{Pa s}$	1.652(26)	0.026 09(16)	$8.42(32) \times 10^{-6}$	$-5.58(19) \times 10^{-9}$
$\rho D/\text{g m}^{-1} \text{ s}^{-1}$	1.165(31)	0.039 50(20)	$3.62(38) \times 10^{-6}$	$-4.43(23) \times 10^{-9}$

TABLE 27. Potential parameters $r_m(T)$ and $\varepsilon(T)$ and recommended thermophysical properties of SiCl_4

T/K	$r_m/10^{-8} \text{ cm}$	$\varepsilon/k_B/\text{K}$	$-B(T)/\text{cm}^3 \text{ mol}^{-1}$	$\eta/\mu\text{Pa s}$	$\rho D/\text{g m}^{-1} \text{ s}^{-1}$
200	5.777 974	725.8397	4280.803 00	7.2124	9.2555
210	5.783 255	721.8719	3666.085 88	7.5067	9.6515
220	5.788 539	717.9277	3182.618 97	7.7994	10.0461
230	5.793 826	714.0055	2794.978 00	8.0910	10.4396
240	5.799 120	710.1039	2478.888 12	8.3815	10.8321
250	5.804 418	706.2239	2217.310 06	8.6710	11.2239
260	5.809 714	702.3698	1998.017 33	8.9595	11.6154
270	5.815 002	698.5460	1812.045 80	9.2477	12.0067
280	5.820 276	694.7567	1652.703 78	9.5360	12.3979
290	5.825 533	691.0038	1514.908 76	9.8249	12.7894
300	5.830 770	687.2882	1394.747 08	10.1146	13.1810
310	5.835 986	683.6107	1289.168 27	10.4051	13.5728
320	5.841 179	679.9721	1195.765 66	10.6965	13.9646
330	5.846 348	676.3731	1112.619 02	10.9887	14.3564
340	5.851 491	672.8143	1038.180 61	11.2817	14.7480
350	5.856 606	669.2964	971.191 17	11.5755	15.1392
360	5.861 692	665.8196	910.616 68	11.8699	15.5300
370	5.866 748	662.3841	855.601 00	12.1650	15.9202
380	5.871 773	658.9897	805.430 42	12.4606	16.3097
390	5.876 768	655.6366	759.505 89	12.7565	16.6984
400	5.881 730	652.3244	717.321 04	13.0526	17.0861
410	5.886 661	649.0530	678.445 35	13.3489	17.4727
420	5.891 559	645.8221	642.510 76	13.6452	17.8583
430	5.896 425	642.6313	609.200 95	13.9418	18.2428
440	5.901 257	639.4803	578.242 51	14.2384	18.6264
450	5.906 057	636.3686	549.398 17	14.5353	19.0091
460	5.910 823	633.2957	522.461 09	14.8323	19.3910
470	5.915 557	630.2612	497.250 18	15.1293	19.7720
480	5.920 257	627.2647	473.606 26	15.4263	20.1523
490	5.924 925	624.3055	451.388 90	15.7230	20.5319
500	5.929 560	621.3831	430.473 80	16.0193	20.9107
510	5.934 163	618.4972	410.750 54	16.3152	21.2888
520	5.938 732	615.6472	392.120 73	16.6104	21.6655
530	5.943 269	612.8326	374.496 43	16.9048	22.0401
540	5.947 774	610.0531	357.798 82	17.1984	22.4120
550	5.952 246	607.3080	341.957 08	17.4910	22.7802
560	5.956 686	604.5972	326.907 41	17.7825	23.1445
570	5.961 093	601.9202	312.592 17	18.0729	23.5055
580	5.965 468	599.2767	298.959 18	18.3624	23.8639
590	5.969 809	596.6664	285.961 13	18.6509	24.2207
600	5.974 118	594.0890	273.554 98	18.9386	24.5769
610	5.978 393	591.5445	261.701 50	19.2255	24.9329
620	5.982 635	589.0325	250.364 92	19.5114	25.2885
630	5.986 843	586.5531	239.512 53	19.7962	25.6434
640	5.991 015	584.1061	229.114 34	20.0799	25.9972
650	5.995 153	581.6914	219.142 82	20.3622	26.3496
660	5.999 255	579.3092	209.572 67	20.6430	26.7003
670	6.003 320	576.9593	200.380 61	20.9222	27.0488
680	6.007 349	574.6419	191.545 15	21.1995	27.3947
690	6.011 339	572.3570	183.046 43	21.4750	27.7374
700	6.015 291	570.1048	174.866 09	21.7483	28.0768
710	6.019 202	567.8854	166.987 15	22.0197	28.4129
720	6.023 074	565.6988	159.393 80	22.2892	28.7459
730	6.026 904	563.5453	152.071 38	22.5569	29.0760
740	6.030 691	561.4250	145.006 18	22.8229	29.4034
750	6.034 436	559.3378	138.185 46	23.0874	29.7284
760	6.038 137	557.2839	131.597 32	23.3505	30.0511
770	6.041 793	555.2635	125.230 72	23.6124	30.3720
780	6.045 404	553.2769	119.075 37	23.8733	30.6912
790	6.048 967	551.3244	113.121 64	24.1331	31.0090
800	6.052 482	549.4060	107.360 43	24.3919	31.3253
810	6.055 949	547.5212	101.782 83	24.6494	31.6400
820	6.059 370	545.6694	96.380 38	24.9055	31.9532
830	6.062 744	543.8499	91.145 15	25.1600	32.2646
840	6.066 070	542.0630	86.070 25	25.4129	32.5742

TABLE 27. Potential parameters $r_m(T)$ and $\varepsilon(T)$ and recommended thermophysical properties of SiCl_4 —Continued

T/K	$r_m/10^{-8}$ cm	$\varepsilon/k_B/\text{K}$	$-B(T)/\text{cm}^3 \text{ mol}^{-1}$	$\eta/\mu\text{Pa s}$	$\rho D/\text{g m}^{-1} \text{ s}^{-1}$
850	6.069 344	540.3110	81.150 17	25.6638	32.8821
860	6.072 560	538.5964	76.379 86	25.9127	33.1880
870	6.075 714	536.9211	71.754 31	26.1594	33.4920
880	6.078 814	535.2804	67.265 43	26.4039	33.7940
890	6.081 876	533.6651	62.902 98	26.6463	34.0940
900	6.084 920	532.0656	58.657 18	26.8867	34.3921

TABLE 28. Fit parameters according to Eqs. (6) and (7) for SiCl_4

Property	A_1	A_2	A_3	A_4
$r_m/10^{-10}$ m	5.665 57(23)	0.000 575 8(14)	$-6.33(28) \times 10^{-8}$	$-6.52(17) \times 10^{-11}$
$\varepsilon/k_B/\text{K}$	816.29(15)	$-0.495 15(98)$	0.000 225 2(19)	$-2.90(11) \times 10^{-8}$
$-B(T)/\text{cm}^3 \text{ mol}^{-1}$	563(21)	$-7.27(27) \times 10^5$	$2.21(10) \times 10^8$	$-5.36(12) \times 10^{10}$
$\eta/\mu\text{Pa s}$	1.854(22)	0.025 00(14)	$1.110(27) \times 10^{-5}$	$-8.89(16) \times 10^{-9}$
$\rho D/\text{g m}^{-1} \text{ s}^{-1}$	1.364(29)	0.038 88(19)	$3.96(36) \times 10^{-6}$	$-7.15(22) \times 10^{-9}$

TABLE 29. Potential parameters $r_m(T)$ and $\varepsilon(T)$ and recommended thermophysical properties of SF_6

T/K	$r_m/10^{-8}$ cm	$\varepsilon/k_B/\text{K}$	$-B/\text{cm}^3 \text{ mol}^{-1}$	$\eta/\mu\text{Pa s}$	$\rho D/\text{g m}^{-1} \text{ s}^{-1}$
170	5.047 029	414.8142	933.877 55	9.3870	12.1653
180	5.048 435	414.1217	821.138 80	9.8480	12.7777
190	5.049 877	413.4128	729.026 15	10.3076	13.3874
200	5.051 332	412.6990	652.533 64	10.7662	13.9942
210	5.053 076	411.8450	587.855 58	11.2240	14.5983
220	5.054 854	410.9766	532.540 35	11.6811	15.1994
230	5.056 695	410.0793	484.832 63	12.1377	16.3927
240	5.058 631	409.1389	443.261 97	12.5937	16.9850
250	5.060 680	408.1457	406.705 53	13.0489	17.5741
260	5.062 834	407.1048	374.306 55	13.5033	18.1597
270	5.065 078	406.0243	345.404 63	13.9568	18.7411
280	5.067 394	404.9120	319.472 15	14.4092	19.3178
290	5.069 770	403.7748	296.081 57	14.8602	19.8900
300	5.072 200	402.6152	274.879 10	15.3100	20.4584
310	5.074 684	401.4346	255.571 51	15.7588	21.0237
320	5.077 217	400.2340	237.915 29	16.2068	21.5866
330	5.079 798	399.0157	221.706 94	16.6541	22.1466
340	5.082 423	397.7809	206.775 58	17.1000	22.7028
350	5.085 080	396.5323	192.976 23	17.5432	23.2543
360	5.087 785	395.2721	180.185 07	17.9822	23.8004
370	5.090 514	394.0025	168.295 44	18.4166	24.3411
380	5.093 269	392.7252	157.214 95	18.8475	24.8766
390	5.096 050	391.4414	146.863 42	19.2760	25.4070
400	5.098 852	390.1525	137.170 94	19.7035	25.9325
410	5.101 672	388.8599	128.076 24	20.1300	26.4533
420	5.104 510	387.5647	119.525 43	20.5549	26.9693
430	5.107 362	386.2682	111.470 92	20.9777	27.4809
440	5.110 225	384.9713	103.870 57	21.3977	27.9883
450	5.113 098	383.6753	96.686 82	21.8141	28.4916
460	5.115 978	382.3811	89.886 19	22.2261	28.9912
470	5.118 864	381.0897	83.438 75	22.6331	29.4868
480	5.121 752	379.8020	77.317 63	23.0353	29.9783
490	5.124 641	378.5193	71.498 68	23.4331	30.4655
500	5.127 529	377.2421	65.960 11	23.8269	30.9480

TABLE 29. Potential parameters $r_m(T)$ and $\varepsilon(T)$ and recommended thermophysical properties of SF₆—Continued

T/K	$r_m/10^{-8}$ cm	$\varepsilon/k_B/K$	$-B(T)/\text{cm}^3 \text{ mol}^{-1}$	$\eta/\mu\text{Pa s}$	$\rho D/\text{g m}^{-1}\text{s}^{-1}$
510	5.130 412	375.9716	60.682 22	24.2174	31.4257
520	5.133 290	374.7087	55.647 21	24.6052	31.8982
530	5.136 159	373.4544	50.838 90	24.9908	31.8982
540	5.139 018	372.2098	46.242 58	25.3744	32.3656
550	5.141 863	370.9758	41.844 82	25.7556	32.8279
560	5.144 692	369.7535	37.633 42	26.1342	33.2853
570	5.1475 03	368.5439	33.597 16	26.5096	33.7380
580	5.150 292	367.3479	29.725 78	26.8815	34.1861
590	5.153 057	366.1666	26.009 86	27.2494	34.6299
600	5.155 796	365.0010	22.440 70	27.6130	35.0696
610	5.158 507	363.8519	19.010 32	27.9726	35.5053
620	5.161 185	362.7200	15.711 32	28.3282	35.9374
630	5.163 830	361.6072	12.536 84	28.6802	36.3659
640	5.166 438	360.5131	9.480 50	29.0286	36.7911
650	5.169 009	359.4389	6.536 41	29.3739	37.2132
660	5.171 538	358.3853	3.699 05	29.7161	37.6324
670	5.174 026	357.3527	0.963 26	30.0553	38.0485
680	5.176 469	356.3418	-1.675 81	30.3916	38.4615
690	5.178 867	355.3529	-4.222 63	30.7248	38.8712
700	5.181 219	354.3865	-6.681 47	31.0551	39.2774
710	5.183 522	353.4427	-9.056 35	31.3825	39.6800
720	5.185 776	352.5217	-11.351 01	31.7070	40.0790
730	5.187 981	351.6237	-13.568 99	32.0287	40.4743
740	5.190 136	350.7488	-15.713 69	32.3477	40.8661
750	5.192 240	349.8968	-17.788 30	32.6639	41.2545
760	5.194 294	349.0676	-19.795 84	32.9775	41.6396
770	5.196 296	348.2612	-21.739 14	33.2885	42.0214
780	5.198 248	347.4773	-23.620 88	33.5970	42.4002
790	5.200 150	346.7157	-25.443 61	33.9032	42.7759
800	5.202 001	345.9760	-27.209 73	34.2070	43.1487
810	5.203 803	345.2577	-28.921 68	34.5086	43.5188
820	5.205 556	344.5606	-30.581 86	34.8080	43.8861
830	5.207 261	343.8843	-32.192 46	35.1052	44.2509
840	5.208 918	343.2285	-33.755 48	35.4005	44.6131
850	5.210 528	342.5926	-35.272 34	35.6938	44.9730
860	5.212 092	341.9763	-36.744 33	35.9851	45.3306
870	5.213 611	341.3790	-38.172 72	36.2744	45.6859
880	5.215 087	340.7997	-39.560 03	36.5619	46.0390
890	5.216 522	340.2377	-40.909 76	36.8473	46.3899
900	5.217 917	339.6924	-42.225 35	37.1307	46.7384
910	5.219 264	339.1666	-43.502 21	37.4123	47.0850
920	5.220 578	338.6546	-44.744 23	37.6921	47.4296
930	5.221 854	338.1583	-45.952 82	37.9699	47.7723
940	5.223 092	337.6780	-47.128 94	38.2459	48.1131
950	5.224 289	337.2140	-48.273 47	38.5201	48.4520
960	5.225 444	336.7669	-49.387 27	38.7926	48.7893
970	5.226 560	336.3356	-50.471 62	39.0633	49.1248
980	5.227 647	335.9165	-51.528 63	39.3323	49.4585
990	5.228 712	335.5058	-52.560 41	39.5995	49.7905
1000	5.229 768	335.0999	-53.569 00	39.8649	50.1206

TABLE 30. Fit parameters according to Eqs. (6) and (7) for SF₆

Property	A_1	A_2	A_3	A_4
$r_m/10^{-10}$ m	5.0244(12)	$5.06(76) \times 10^{-5}$	$4.67(14) \times 10^{-7}$	$-3.148(80) \times 10^{-10}$
$\varepsilon/k_B/K$	428.84(67)	-0.0505(42)	-0.000 166 6(77)	$1.245(44) \times 10^{-7}$
$-B(T)/\text{cm}^3 \text{ mol}^{-1}$	162.8(1.1)	$-1.053(14) \times 10^5$	$1.1(4.8) \times 10^5$	$-2.347(51) \times 10^9$
$\eta/\mu\text{Pa s}$	0.573(27)	0.053 66(10)	$-1.4455(86) \times 10^{-5}$	—
$\rho D/\text{g m}^{-1}\text{s}^{-1}$	-0.77(18)	0.0845(11)	$-5.18(21) \times 10^{-5}$	$1.84(12) \times 10^{-8}$

TABLE 31. Potential parameters $r_m(T)$ and $\varepsilon(T)$ and recommended thermophysical properties of MoF₆

T/K	$r_m/10^{-8}$ cm	$\varepsilon/k_B/K$	$-B(T)/\text{cm}^3 \text{ mol}^{-1}$	$\eta/\mu\text{Pa s}$	$\rho D/\text{g m}^{-1} \text{ s}^{-1}$
200	5.088 801	739.9354	3005.182 35	10.3388	13.2588
210	5.096 166	733.5425	2547.437 34	10.7593	13.8234
220	5.103 534	727.2111	2191.585 79	11.1771	14.3861
230	5.110 908	720.9380	1909.157 58	11.5930	14.9468
240	5.118 292	714.7202	1680.912 76	12.0071	15.5062
250	5.125 683	708.5586	1493.518 40	12.4200	16.0646
260	5.133 075	702.4591	1337.518 60	12.8319	16.6224
270	5.140 458	696.4274	1206.050 37	13.2435	17.1800
280	5.147 825	690.4688	1094.037 36	13.6554	17.7377
290	5.155 171	684.5857	997.655 15	14.0682	18.2955
300	5.162 496	678.7785	913.981 36	14.4820	18.8536
310	5.169 796	673.0477	840.755 03	14.8970	19.4118
320	5.177 070	667.3938	776.204 45	15.3133	19.9700
330	5.184 315	661.8171	718.924 98	15.7309	20.5280
340	5.191 530	656.3179	667.791 05	16.1498	21.0856
350	5.198 712	650.8964	621.891 84	16.5699	21.6426
360	5.205 860	645.5525	580.483 16	16.9911	22.1988
370	5.212 972	640.2858	542.951 64	17.4133	22.7541
380	5.220 049	635.0958	508.788 24	17.8362	23.3082
390	5.227 087	629.9817	477.567 42	18.2596	23.8609
400	5.234 088	624.9430	448.930 95	18.6833	24.4119
410	5.241 049	619.9791	422.575 37	19.1075	24.9614
420	5.247 971	615.0891	398.242 13	19.5320	25.5091
430	5.254 852	610.2724	375.709 77	19.9568	26.0550
440	5.261 691	605.5285	354.787 66	20.3819	26.5991
450	5.268 487	600.8569	335.310 85	20.8071	27.1416
460	5.275 239	596.2571	317.135 91	21.2324	27.6826
470	5.281 946	591.7286	300.137 76	21.6576	28.2225
480	5.288 606	587.2717	284.207 00	22.0825	28.7615
490	5.295 217	582.8864	269.247 34	22.5067	29.2987
500	5.301 777	578.5728	255.173 71	22.9298	29.8330
510	5.308 282	574.3313	241.910 99	23.3510	30.3629
520	5.314 731	570.1629	229.392 56	23.7697	30.8867
530	5.321 119	566.0683	217.559 00	24.1857	31.4040
540	5.327 443	562.0485	206.357 14	24.5995	31.9163
550	5.333 699	558.1046	195.739 52	25.0116	32.4250
560	5.339 882	554.2380	185.663 52	25.4226	32.9318
570	5.345 989	550.4500	176.090 67	25.8328	33.4376
580	5.352 015	546.7420	166.986 21	26.2418	33.9420
590	5.357 955	543.1153	158.318 68	26.6493	34.4445
600	5.363 805	539.5711	150.059 49	27.0548	34.9445
610	5.369 559	536.1109	142.182 62	27.4578	35.4415
620	5.375 214	532.7356	134.664 26	27.8580	35.9347
630	5.380 766	529.4460	127.482 51	28.2546	36.4235
640	5.386 211	526.2430	120.617 34	28.6473	36.9071
650	5.391 544	523.1272	114.050 36	29.0358	37.3854
660	5.396 764	520.0989	107.764 41	29.4206	37.8586
670	5.401 867	517.1578	101.743 61	29.8018	38.3270
680	5.406 851	514.3040	95.973 33	30.1800	38.7911
690	5.411 714	511.5372	90.439 97	30.5555	39.2511
700	5.416 455	508.8567	85.130 71	30.9287	39.7076
710	5.421 073	506.2614	80.033 62	31.3002	40.1609
720	5.425 567	503.7505	75.137 67	31.6702	40.6115
730	5.429 937	501.3229	70.432 43	32.0386	41.0593
740	5.434 184	498.9767	65.908 01	32.4050	41.5044
750	5.438 309	496.7103	61.555 19	32.7692	41.9465
760	5.442 312	494.5222	57.365 36	33.1309	42.3856
770	5.446 195	492.4106	53.330 47	33.4896	42.8216
780	5.449 959	490.3737	49.442 94	33.8450	43.2544
790	5.453 605	488.4099	45.695 69	34.1968	43.6840
800	5.457 135	486.5172	42.081 98	34.5450	44.1104
810	5.460 554	484.6927	38.595 02	34.8898	44.5337
820	5.463 865	482.9329	35.228 29	35.2314	44.9539
830	5.467 073	481.2349	31.975 70	35.5700	45.3713
840	5.470 181	479.5970	28.832 15	35.9059	45.7859

TABLE 31. Potential parameters $r_m(T)$ and $\varepsilon(T)$ and recommended thermophysical properties of MoF₆—Continued

T/K	$r_m/10^{-8}$ cm	$\varepsilon/k_B/K$	$-B(T)/\text{cm}^3 \text{ mol}^{-1}$	$\eta/\mu\text{Pa s}$	$\rho D/\text{g m}^{-1} \text{ s}^{-1}$
850	5.473 182	478.0210	25.794 05	36.2393	46.1979
860	5.476 074	476.5087	22.858 12	36.5705	46.6075
870	5.478 851	475.0612	20.021 03	36.8997	47.0147
880	5.481 530	473.6696	17.275 73	37.2270	47.4194
890	5.484 143	472.3172	14.612 49	37.5521	47.8216
900	5.486 721	470.9872	12.021 99	37.8751	48.2210

TABLE 32. Fit parameters according to Eqs. (6) and (7) for MoF₆

Property	A_1	A_2	A_3	A_4
$r_m/10^{-10}$ m	4.9467 1(75)	0.000 671 1(48)	$2.784(93) \times 10^{-7}$	$-3.987(56) \times 10^{-10}$
$\varepsilon/k_B/K$	884.00(43)	-0.7891(27)	0.000 341 6(53)	$2.90(32) \times 10^{-8}$
$-B(T)/\text{cm}^3 \text{ mol}^{-1}$	440(19)	$-5.45(24) \times 10^5$	$1.818(92) \times 10^8$	$-4.18(11) \times 10^{10}$
$\eta/\mu\text{Pa s}$	2.691(51)	0.035 30(32)	$1.801(62) \times 10^{-5}$	$-1.540(38) \times 10^{-10}$
$\rho D/\text{g m}^{-1} \text{ s}^{-1}$	1.758(74)	0.056 99(47)	$3.50(92) \times 10^{-7}$	$-1.062(55) \times 10^{-8}$

TABLE 33. Potential parameters $r_m(T)$ and $\varepsilon(T)$ and recommended thermophysical properties of WF₆

T/K	$r_m/10^{-8}$ cm	$\varepsilon/k_B/K$	$-B(T)/\text{cm}^3 \text{ mol}^{-1}$	$\eta/\mu\text{Pa s}$	$\rho D/\text{g m}^{-1} \text{ s}^{-1}$
200	5.180 392	630.8432	2484.050 91	11.8364	15.3056
210	5.191 169	623.0266	2135.424 29	12.3409	16.0051
220	5.201 983	615.2954	1859.263 41	12.8420	16.7056
230	5.212 872	607.6243	1636.213 37	13.3387	17.4070
240	5.223 868	599.9901	1452.976 79	13.8377	18.1138
250	5.234 979	592.3898	1300.251 73	14.3464	18.8306
260	5.246 176	584.8444	1171.393 88	14.8668	19.5581
270	5.257 426	577.3752	1061.494 24	15.3982	20.2956
280	5.268 701	570.0015	966.856 69	15.9397	21.0412
290	5.279 986	562.7309	884.634 47	16.4894	21.7927
300	5.291 276	555.5651	812.614 69	17.0461	22.5483
310	5.302 566	548.5054	749.066 01	17.6089	23.3065
320	5.313 851	541.5533	692.617 99	18.1765	24.0655
330	5.325 124	534.7109	642.174 84	18.7470	24.8233
340	5.336 378	527.9803	596.850 45	19.3201	25.5797
350	5.347 607	521.3633	555.921 33	19.8960	26.3363
360	5.358 804	514.8610	518.790 64	20.4756	27.0955
370	5.369 967	508.4728	484.961 54	21.0590	27.8594
380	5.381 091	502.1984	454.018 66	21.6439	28.6260
390	5.392 174	496.0370	425.612 47	22.2262	29.3919
400	5.403 212	489.9878	399.446 67	22.8014	30.1526
410	5.414 203	484.0497	375.268 65	23.3711	30.9061
420	5.425 145	478.2216	352.862 00	23.9435	31.6530
430	5.436 035	472.5024	332.040 30	24.5293	32.3949
440	5.446 870	466.8909	312.642 13	25.1324	33.1329
450	5.457 648	461.3858	294.527 11	25.7418	33.8677
460	5.468 367	455.9860	277.572 64	26.3425	34.5995
470	5.479 024	450.6903	261.671 32	26.9233	35.3281
480	5.489 616	445.4980	246.728 87	27.4859	36.0526
490	5.500 139	440.4083	232.661 96	28.0345	36.7720
500	5.510 590	435.4205	219.396 75	28.5744	37.4853

TABLE 33. Potential parameters $r_m(T)$ and $\varepsilon(T)$ and recommended thermophysical properties of WF₆ —Continued

T/K	$r_m/10^{-8}$ cm	$\varepsilon/k_B/K$	$-B(T)/\text{cm}^3 \text{ mol}^{-1}$	$\eta/\mu\text{Pa s}$	$\rho D/\text{g m}^{-1} \text{ s}^{-1}$
510	5.520 964	430.5343	206.867 80	29.1122	38.1916
520	5.531 257	425.7496	195.017 00	29.6554	38.8900
530	5.541 464	421.0663	183.792 32	30.2060	39.5799
540	5.551 578	416.4845	173.147 08	30.7606	40.2605
550	5.561 593	412.0045	163.039 60	31.3146	40.9314
560	5.571 504	407.6269	153.432 37	31.8629	41.5920
570	5.581 302	403.3521	144.291 47	32.3996	42.2415
580	5.590 981	399.1806	135.586 16	32.9214	42.8804
590	5.600 533	395.1129	127.288 62	33.4296	43.5104
600	5.609 951	391.1497	119.373 54	33.9266	44.1340
610	5.619 227	387.2913	111.817 81	34.4152	44.7539
620	5.628 355	383.5380	104.600 24	34.8985	45.3731
630	5.637 328	379.8899	97.701 29	35.3783	45.9925
640	5.646 138	376.3470	91.103 08	35.8544	46.6098
650	5.654 780	372.9092	84.789 12	36.3262	47.2222
660	5.663 248	369.5761	78.743 97	36.7934	47.8265
670	5.671 538	366.3467	72.953 26	37.2553	48.4196
680	5.679 645	363.2204	67.403 74	37.7121	49.0010
690	5.687 565	360.1962	62.083 05	38.1640	49.5719
700	5.695 296	357.2725	56.979 44	38.6115	50.1339
710	5.702 835	354.4479	52.081 92	39.0549	50.6885
720	5.710 181	351.7208	47.380 32	39.4947	51.2372
730	5.717 333	349.0893	42.864 98	39.9307	51.7802
740	5.724 291	346.5511	38.526 60	40.3625	52.3178
750	5.731 055	344.1040	34.356 50	40.7899	52.8501
760	5.737 628	341.7457	30.346 58	41.2126	53.3773
770	5.744 009	339.4740	26.489 22	41.6303	53.8996
780	5.750 201	337.2866	22.777 21	42.0427	54.4173
790	5.756 205	335.1814	19.203 82	42.4496	54.9305
800	5.762 023	333.1558	15.762 60	42.8506	55.4396
810	5.767 662	331.2064	12.446 80	43.2455	55.9448
820	5.773 128	329.3292	9.249 90	43.6348	56.4462
830	5.778 429	327.5208	6.165 79	44.0189	56.9439
840	5.783 565	325.7793	3.189 62	44.3984	57.4381
850	5.788 531	324.1060	0.318 41	44.7738	57.9289
860	5.793 318	322.5020	-2.450 47	45.1457	58.4166
870	5.797 919	320.9701	-5.119 86	45.5148	58.9013
880	5.802 360	319.4988	-7.697 79	45.8816	59.3831
890	5.806 693	318.0710	-10.196 08	46.2464	59.8618
900	5.810 969	316.6692	-12.626 14	46.6095	60.3372

TABLE 34. Fit parameters according to Eqs. (6) and (7) for WF₆

Property	A_1	A_2	A_3	A_4
$r_m/10^{-10}$ m	4.9734(12)	0.000 928 4(77)	$6.58(15) \times 10^{-7}$	$-7.315(90) \times 10^{-10}$
$\varepsilon/k_B/K$	819.91(64)	-1.0619(41)	0.000 619 1(79)	$-6.62(47) \times 10^{-8}$
$-B(T)/\text{cm}^3 \text{ mol}^{-1}$	365(12)	$-3.90(16) \times 10^5$	$1.042(59) \times 10^8$	$-2.785(69) \times 10^{10}$
$\eta/\mu\text{Pa s}$	1.47(26)	0.0453(17)	$3.27(32) \times 10^{-5}$	$-3.07(19) \times 10^{-8}$
$\rho D/\text{g m}^{-1} \text{ s}^{-1}$	-0.42(28)	0.0760(18)	$1.04(34) \times 10^{-5}$	$-2.23(20) \times 10^{-8}$

TABLE 35. Potential parameters $r_m(T)$ and $\varepsilon(T)$ and recommended thermophysical properties of UF_6

T/K	$r_m/10^{-8} \text{ cm}$	$\varepsilon/k_B/\text{K}$	$-B(T)/\text{cm}^3 \text{ mol}^{-1}$	$\eta/\mu\text{Pa s}$	$\rho D/\text{g m}^{-1} \text{ s}^{-1}$
200	5.130 224	82.88266	5555.013 24	12.4449	15.8793
210	5.140 778	872.0077	4508.327 56	12.9493	16.5496
220	5.151 313	861.3616	3735.454 65	13.4490	17.2173
230	5.161 814	850.9016	3149.861 15	13.9449	17.8834
240	5.172 262	840.6400	2696.067 97	14.4375	18.5479
250	5.182 649	830.5818	2337.357 90	14.9276	19.2109
260	5.192 973	820.7235	2048.758 09	15.4159	19.8724
270	5.203 233	811.0612	1812.904 65	15.9028	20.5328
280	5.213 428	801.5913	1617.457 15	16.3886	21.1928
290	5.223 557	792.3105	1453.470 86	16.8737	21.8527
300	5.233 617	783.2164	1314.343 46	17.3587	22.5130
310	5.243 606	774.3063	1195.120 30	17.8444	23.1740
320	5.253 524	765.5774	1092.026 80	18.3317	23.8358
330	5.263 368	757.0258	1002.146 37	18.8208	24.4985
340	5.273 140	748.6476	923.198 86	19.3119	25.1620
350	5.282 839	740.4388	853.381 56	19.8052	25.8262
360	5.292 464	732.3957	791.253 92	20.3005	26.4909
370	5.302 016	724.5143	735.653 39	20.7980	27.1556
380	5.311 495	716.7908	685.633 39	21.2975	27.8201
390	5.320 902	709.2217	640.416 70	21.7988	28.4841
400	5.330 234	701.8034	599.360 15	22.3019	29.1475
410	5.339 494	694.5325	561.927 61	22.8064	29.8099
420	5.348 681	687.4059	527.669 09	23.3119	30.4709
430	5.357 794	680.4203	496.204 58	23.8182	31.1303
440	5.366 833	673.5733	467.211 70	24.3253	31.7880
450	5.375 796	666.8628	440.415 07	24.8332	32.4439
460	5.384 683	660.2865	415.578 06	25.3418	33.0978
470	5.393 492	653.8427	392.496 70	25.8510	33.7498
480	5.402 219	647.5305	370.994 77	26.3607	34.4000
490	5.410 862	641.3493	350.918 71	26.8707	35.0486
500	5.419 417	635.2984	332.134 14	27.3808	35.6958
510	5.427 881	629.3776	314.523 53	27.8907	36.3421
520	5.436 249	623.5876	297.983 66	28.4001	36.9868
530	5.444 514	617.9290	282.423 15	28.9083	37.6283
540	5.452 673	612.4022	267.760 87	29.4145	38.2647
550	5.460 718	607.0083	253.924 87	29.9178	38.8938
560	5.468 645	601.7484	240.850 94	30.4178	39.5145
570	5.476 446	596.6235	228.481 55	30.9150	40.1283
580	5.484 116	591.6345	216.764 93	31.4099	40.7372
590	5.491 649	586.7821	205.654 37	31.9033	41.3435
600	5.499 038	582.0669	195.107 64	32.3956	41.9488
610	5.506 279	577.4894	185.086 56	32.8865	42.5528
620	5.513 366	573.0497	175.556 19	33.3754	43.1547
630	5.520 296	568.7473	166.484 49	33.8619	43.7538
640	5.527 063	564.5817	157.842 27	34.3454	44.3494
650	5.533 665	560.5522	149.602 88	34.8253	44.9405
660	5.540 099	556.6575	141.741 47	35.3010	45.5262
670	5.546 364	552.8956	134.235 07	35.7719	46.1056
680	5.552 458	549.2649	127.062 62	36.2378	46.6784
690	5.558 379	545.7633	120.204 69	36.6990	47.2448
700	5.564 129	542.3880	113.642 92	37.1559	47.8053
710	5.569 708	539.1364	107.360 34	37.6090	48.3605
720	5.575 117	536.0057	101.341 29	38.0588	48.9107
730	5.580 357	532.9928	95.571 08	38.5057	49.4567
740	5.585 431	530.0941	90.035 82	38.9505	49.9989
750	5.590 342	527.3062	84.722 61	39.3934	50.5379
760	5.595 093	524.6256	79.619 48	39.8345	51.0738
770	5.599 686	522.0491	74.715 24	40.2734	51.6066
780	5.604 124	519.5732	69.999 50	40.7098	52.1360
790	5.608 411	517.1949	65.462 52	41.1432	52.6621
800	5.612 550	514.9107	61.095 10	41.5734	53.1847
810	5.616 547	512.7160	56.888 04	41.9998	53.7037
820	5.620 409	510.6060	52.832 56	42.4222	54.2190
830	5.624 142	508.5758	48.920 45	42.8403	54.7305
840	5.627 749	506.6231	45.144 93	43.2543	55.2385

TABLE 35. Potential parameters $r_m(T)$ and $\varepsilon(T)$ and recommended thermophysical properties of UF_6 —Continued

T/K	$r_m/10^{-8}$ cm	$\varepsilon/k_B/\text{K}$	$-B(T)/\text{cm}^3 \text{ mol}^{-1}$	$\eta/\mu\text{Pa s}$	$\rho D/\text{g m}^{-1} \text{ s}^{-1}$
850	5.631 226	504.7492	41.501 21	43.6645	55.7429
860	5.634 567	502.9559	37.984 98	44.0711	56.2440
870	5.637 770	501.2439	34.591 84	44.4745	56.7419
880	5.640 854	499.6020	31.312 48	44.8749	57.2368
890	5.643 857	498.0091	28.134 09	45.2725	57.7286
900	5.646 818	496.4445	25.044 39	45.6675	58.2174

TABLE 36. Fit parameters according to Eqs. (6) and (7) for UF_6

Property	A_1	A_2	A_3	A_4
$r_m/10^{-10}$ m	4.9186(13)	0.001 055 6(85)	$1.06(16) \times 10^{-7}$	$-4.245(99) \times 10^{-10}$
$\varepsilon/k_B/\text{K}$	1133.60(73)	$-1.4506(46)$	0.001 007 4(90)	$-2.017(54) \times 10^{-7}$
$-B(T)/\text{cm}^3 \text{ mol}^{-1}$	1033(67)	$-1.460(84) \times 10^6$	$6.20(32) \times 10^8$	$-1.172(37) \times 10^{11}$
$\eta/\mu\text{Pa s}$	3.907(67)	0.038 30(43)	$2.783(82) \times 10^{-5}$	$-2.099(50) \times 10^{-8}$
$\rho D/\text{g m}^{-1} \text{ s}^{-1}$	2.756(91)	0.063 49(58)	$1.33(11) \times 10^{-5}$	$-1.725(68) \times 10^{-8}$

TABLE 37. Potential parameters $r_m(T)$ and $\varepsilon(T)$ and recommended thermophysical properties of $\text{C}(\text{CH}_3)_4$

T/K	$r_m/10^{-8}$ cm	$\varepsilon/k_B/\text{K}$	$-B(T)/\text{cm}^3 \text{ mol}^{-1}$	$\eta/\mu\text{Pa s}$	$\rho D/\text{g m}^{-1} \text{ s}^{-1}$
200	5.803 668	571.5110	2216.836 30	5.0650	6.5499
210	5.806 938	569.5832	1958.779 72	5.2748	6.8325
220	5.810 213	567.6591	1746.933 23	5.4840	7.1145
230	5.813 502	565.7349	1570.393 66	5.6930	7.3960
240	5.816 811	563.8068	1421.330 33	5.9020	7.6772
250	5.820 146	561.8712	1293.999 62	6.1112	7.9581
260	5.823 514	559.9244	1184.108 85	6.3207	8.2386
270	5.826 921	557.9629	1088.395 30	6.5305	8.5187
280	5.830 374	555.9830	1004.341 18	6.7405	8.7983
290	5.833 880	553.9815	929.976 74	6.9509	9.0774
300	5.837 445	551.9547	863.741 66	7.1615	9.3559
310	5.841 073	549.9006	804.388 07	7.3723	9.6337
320	5.844 763	547.8210	750.913 86	7.5833	9.9107
330	5.848 510	545.7186	702.500 99	7.7944	10.1870
340	5.852 309	543.5964	658.474 11	8.0054	10.4622
350	5.856 157	541.4571	618.271 20	8.2164	10.7366
360	5.860 048	539.3035	581.421 13	8.4274	11.0100
370	5.863 978	537.1382	547.526 23	8.6384	11.2823
380	5.867 944	534.9639	516.248 73	8.8493	11.5537
390	5.871 940	532.7832	487.300 00	9.0602	11.8242
400	5.875 962	530.5987	460.432 07	9.2710	12.0937
410	5.880 007	528.4125	435.430 34	9.4816	12.3625
420	5.884 073	526.2252	412.106 89	9.6920	12.6306
430	5.888 161	524.0373	390.297 58	9.9021	12.8981
440	5.892 269	521.8490	369.858 80	10.1118	13.1646
450	5.896 397	519.6607	350.664 38	10.3209	13.4296
460	5.900 545	517.4725	332.603 06	10.5290	13.6925
470	5.904 713	515.2850	315.576 34	10.7360	13.9527
480	5.908 899	513.0982	299.496 75	10.9418	14.2100
490	5.913 105	510.9126	284.286 32	11.1466	14.4649
500	5.917 329	508.7284	269.875 37	11.3506	14.7182

TABLE 37. Potential parameters $r_m(T)$ and $\varepsilon(T)$ and recommended thermophysical properties of $C(CH_3)_4$ —Continued

T/K	$r_m/10^{-8}$ cm	$\varepsilon/k_B/K$	$-B(T)/cm^3\ mol^{-1}$	$\eta/\mu\text{Pa s}$	$\rho D/g\ m^{-1}\ s^{-1}$
510	5.921 570	506.5460	256.201 50	11.5540	14.9704
520	5.925 828	504.3659	243.208 82	11.7569	15.2221
530	5.930 102	502.1889	230.847 04	11.9594	15.4731
540	5.934 390	500.0157	219.070 68	12.1611	15.7233
550	5.938 691	497.8468	207.838 54	12.3620	15.9723
560	5.943 004	495.6830	197.113 21	12.5618	16.2200
570	5.947 328	493.5248	186.860 65	12.7603	16.4661
580	5.951 661	491.3729	177.049 81	12.9574	16.7102
590	5.956 002	489.2278	167.652 32	13.1528	16.9521
600	5.960 350	487.0903	158.642 21	13.3464	17.1914
610	5.964 705	484.9607	149.995 60	13.5381	17.4283
620	5.969 064	482.8394	141.69044	13.7282	17.6628
630	5.973 428	480.7266	133.706 36	13.9168	17.8951
640	5.977 797	478.6227	126.024 61	14.1040	18.1253
650	5.982 169	476.5277	118.627 87	14.2900	18.3537
660	5.986 544	474.4420	111.500 11	14.4751	18.5804
670	5.990 922	472.3657	104.626 51	14.6594	18.8056
680	5.995 301	470.2991	97.993 31	14.8429	19.0293
690	5.999 682	468.2424	91.587 74	15.0255	19.2516
700	6.004 064	466.1957	85.397 92	15.2070	19.4724
710	6.008 446	464.1594	79.412 82	15.3872	19.6915
720	6.012 828	462.1337	73.622 17	15.5660	19.9089
730	6.017 208	460.1189	68.016 44	15.7430	20.1246
740	6.021 586	458.1153	62.586 70	15.9182	20.3385
750	6.025 961	456.1232	57.324 60	16.0913	20.5505
760	6.030 333	454.1428	52.222 32	16.2626	20.7607
770	6.034 700	452.1745	47.272 55	16.4320	20.9691
780	6.039 062	450.2185	42.468 41	16.5997	21.1757
790	6.043 417	448.2751	37.803 46	16.7659	21.3807
800	6.047 766	446.3445	33.271 63	16.9306	21.5840
810	6.052 108	444.4269	28.867 16	17.0940	21.7858
820	6.056 442	442.5219	24.584 35	17.2561	21.9860
830	6.060 770	440.6291	20.417 79	17.4170	22.1845
840	6.065 093	438.7481	16.362 35	17.5765	22.3813
850	6.069 411	436.8785	12.413 20	17.7347	22.5764
860	6.073 726	435.0198	8.565 78	17.8915	22.7696
870	6.078 037	433.1716	4.815 76	18.0469	22.9609
880	6.082 346	431.3336	1.159 05	18.2009	23.1504
890	6.086 654	429.5053	-2.408 23	18.3534	23.3379
900	6.090 961	427.6863	-5.889 76	18.5045	23.5235

TABLE 38. Fit parameters according to Eqs. (6) and (7) for $C(CH_3)_4$

Property	A_1	A_2	A_3	A_4
$r_m/10^{-10}$ m	5.750 79(43)	0.000 199 9(27)	$3.512(53)\times 10^{-7}$	$-1.709(32)\times 10^{-10}$
$\varepsilon/k_B/K$	606.24(35)	-0.1480(22)	-0.000 140 9(43)	$9.48(26)\times 10^{-8}$
$-B(T)/cm^3\ mol^{-1}$	349.0(4.4)	$-3.384(55)\times 10^5$	$4.69(21)\times 10^7$	$-1.630(24)\times 10^{10}$
$\eta/\mu\text{Pa s}$	0.950(19)	0.019 74(12)	$5.09(23)\times 10^{-6}$	$-5.97(14)\times 10^{-9}$
$\rho D/g\ m^{-1}\ s^{-1}$	0.627(23)	0.030 05(15)	$-2.04(28)\times 10^{-6}$	$-3.46(17)\times 10^{-9}$

TABLE 39. Potential parameters $r_m(T)$ and $\varepsilon(T)$ and recommended thermophysical properties of $\text{Si}(\text{CH}_3)_4$

T/K	$r_m/10^{-8} \text{ cm}$	$\varepsilon/k_B/\text{K}$	$-B(T)/\text{cm}^3 \text{ mol}^{-1}$	$\eta/\mu\text{Pa s}$	$\rho D/\text{g m}^{-1} \text{ s}^{-1}$
200	6.011 879	605.9673	3215.343 66	4.9755	6.4355
210	6.020 295	600.9023	2798.903 78	5.1841	6.7213
220	6.028 712	595.8862	2463.764 91	5.3915	7.0072
230	6.037 131	590.9181	2189.402 49	5.5985	7.2937
240	6.045 551	585.9972	1961.412 77	5.8067	7.5814
250	6.053 973	581.1225	1769.451 78	6.0169	7.8708
260	6.062 399	576.2932	1605.936 97	6.2294	8.1618
270	6.070 829	571.5084	1465.206 88	6.4439	8.4542
280	6.079 264	566.7674	1342.963 93	6.6603	8.7478
290	6.087 703	562.0693	1235.896 69	6.8785	9.0421
300	6.096 149	557.4133	1141.418 82	7.0981	9.3368
310	6.104 601	552.7989	1057.485 60	7.3190	9.6316
320	6.113 057	548.2263	982.463 58	7.5409	9.9263
330	6.121 518	543.6955	915.032 98	7.7636	10.2204
340	6.129 982	539.2070	854.116 97	7.9867	10.5138
350	6.138 447	534.7608	798.829 22	8.2104	10.8065
360	6.146 912	630.3573	748.434 28	8.4348	11.0990
370	6.155 377	525.9966	702.317 31	8.6599	11.3917
380	6.163 838	521.6789	659.960 72	8.8858	11.6848
390	6.172 297	517.4042	620.925 95	9.1121	11.9781
400	6.180 750	513.1729	584.839 18	9.3381	12.2712
410	6.189 197	508.9848	551.379 90	9.5633	12.5637
420	6.197 637	504.8401	520.271 69	9.7874	12.8549
430	6.206 069	500.7384	491.275 16	10.0108	13.1443
440	6.214 493	496.6799	464.182 01	10.2347	13.4311
450	6.222 907	492.6642	438.810 22	10.4599	13.7144
460	6.231 310	488.6914	415.000 07	10.6866	13.9943
470	6.239 701	484.7612	392.610 86	10.9137	14.2719
480	6.248 081	480.8735	371.518 19	11.1396	14.5485
490	6.256 447	477.0282	351.611 69	11.3629	14.8254
500	6.264 799	473.2251	332.793 10	11.5833	15.1025
510	6.273 136	469.4641	314.974 67	11.8013	15.3793
520	6.281 458	465.7448	298.077 73	12.0169	15.6551
530	6.289 763	462.0670	282.031 61	12.2306	15.9292
540	6.298 052	458.4304	266.772 66	12.4430	16.2007
550	6.306 323	459.8348	252.243 42	12.6545	16.4689
560	6.314 575	451.2798	238.391 87	12.8655	16.7330
570	6.322 809	447.7652	225.170 84	13.0758	16.9933
580	6.331 023	444.2907	212.537 43	13.2851	17.2499
590	6.339 218	440.8560	200.452 55	13.4932	17.5034
600	6.347 391	437.4608	188.880 51	13.6997	17.7542
610	6.355 543	434.1048	177.788 62	13.9042	18.0026
620	6.363 674	430.7876	167.146 78	14.1064	18.2493
630	6.371 783	427.5085	156.927 32	14.3062	18.4943
640	6.379 871	424.2671	147.104 77	14.5036	18.7375
650	6.387 937	421.0629	137.655 70	14.6986	18.9790
660	6.395 982	417.8953	128.558 46	14.8912	19.2189
670	6.404 005	414.7639	119.793 05	15.0815	19.4571
680	6.412 006	411.6681	111.340 98	15.2694	19.6937
690	6.419 985	408.6076	103.185 05	15.4551	19.9284
700	6.427 943	405.5818	95.309 39	15.6386	20.1609
710	6.435 879	405.903	87.699 22	15.8202	20.3909
720	6.443 792	399.6331	80.341 06	15.9999	20.6180
730	6.451 681	396.7101	73.222 39	16.1779	20.8420
740	6.459 545	393.8212	66.331 51	16.3543	21.0628
750	6.467 382	390.9665	59.657 52	16.5288	21.2807
760	6.475 192	388.1458	53.190 21	16.7017	21.4956
770	6.482 973	385.3591	46.920 05	16.8727	21.7077
780	6.490 723	382.6063	40.838 07	17.0419	21.9171
790	6.498 443	379.8873	34.935 90	17.2093	22.1238
800	6.506 130	377.2021	29.205 65	17.3748	22.3281
810	6.513 785	374.5504	23.639 74	17.5383	22.5299
820	6.521 409	371.9306	18.230 27	17.7000	22.7294
830	6.529 007	369.3413	12.969 63	17.8596	22.9266
840	6.536 581	366.7809	7.850 62	18.0172	23.1217

TABLE 39. Potential parameters $r_m(T)$ and $\varepsilon(T)$ and recommended thermophysical properties of $\text{Si}(\text{CH}_3)_4$ —Continued

T/K	$r_m/10^{-8}$ cm	$\varepsilon/k_B/\text{K}$	$-B(T)/\text{cm}^3 \text{ mol}^{-1}$	$\eta/\mu\text{Pa s}$	$\rho D/\text{g m}^{-1} \text{ s}^{-1}$
850	6.544 135	364.2480	2.866 47	18.1728	23.3148
860	6.551 672	361.7409	−1.989 23	18.3263	23.5060
870	6.559 196	359.2584	−6.722 54	18.4778	23.6956
880	6.566 710	356.7990	−11.339 20	18.6271	23.8836
890	6.574 217	354.3613	−15.844 63	18.7743	24.0700
900	6.581 721	351.9442	−20.243 99	18.9196	24.2546

TABLE 40. Fit parameters according to Eqs. (6) and (7) for $\text{Si}(\text{CH}_3)_4$

Property	A_1	A_2	A_3	A_4
$r_m/10^{-10}$ m	5.844 80(27)	0.000 820 7(17)	$8.91(33) \times 10^{-8}$	$-1.018(20) \times 10^{-10}$
$\varepsilon/k_B/\text{K}$	718.41(17)	−0.6134(11)	0.000 2675(21)	$-4.24(13) \times 10^{-8}$
$-B(T)/\text{cm}^3 \text{ mol}^{-1}$	516(10)	$-5.31(13) \times 10^5$	$1.158(48) \times 10^8$	$-3.163(56) \times 10^{10}$
$\eta/\mu\text{Pa s}$	0.956(50)	0.017 93(32)	$1.200(62) \times 10^{-5}$	$-1.090(37) \times 10^{-8}$
$\rho D/\text{g m}^{-1} \text{ s}^{-1}$	0.452(49)	0.029 06(31)	$4.66(60) \times 10^{-6}$	$-8.47(36) \times 10^{-9}$

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